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(ARLPSU) **TECHNICAL REPORT**

The Pennsylvania State University
APPLIED RESEARCH LABORATORY
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DEVELOPMENT OF A DATABASE OF
THERMOCHEMICAL PARAMETERS FOR USE WITH
THE SOLGASMIX COMPUTER PROGRAM

by

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Technical Report No. TR 88-008

July 1988

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6a. NAME OF PERFORMING ORGANIZATION	6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION
Applied Research Laboratory The Pennsylvania State University	ARL	Naval Sea Systems Command Department of the Navy

6c. ADDRESS (City, State, and ZIP Code)	7b. ADDRESS (City, State, and ZIP Code)
P. O. Box 30 State College, PA 16804	Washington, DC 20362

8a. NAME OF FUNDING / SPONSORING ORGANIZATION	8b. OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
Naval Sea Systems Command	NAVSEA	

8c. ADDRESS (City, State, and ZIP Code)	10. SOURCE OF FUNDING NUMBERS			
Department of the Navy Washington, DC 20362	PROGRAM ELEMENT NO.	PROJECT NO	TASK NO.	WORK UNIT ACCESSION NO.

11. TITLE (Include Security Classification)
Development of a Database of Thermochemical Parameters for Use With the SOLGASMIX Computer Program

12. PERSONAL AUTHOR(S)
Jonathan A. Peters

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
M.S. Thesis	FROM _____ TO _____	July 1988	127

16. SUPPLEMENTARY NOTATION

17.	COSATI CODES		18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	chemical equilibria, SOLGASMIX code, thermochemical analysis, thermodynamic equilibria

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

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20. DISTRIBUTION / AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION
☒ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ☐ DTIC USERS	Unclassified

22a. NAME OF RESPONSIBLE INDIVIDUAL	22b. TELEPHONE (Include Area Code)	22c. OFFICE SYMBOL

presented in detail, and the results of the program compared with those of other methods. Several additional programs, which allow the user to incorporate the curvefit database in other applications, are described. A number of input examples are given for the each of the various programs, and data punching guides are given where appropriate. The various operating systems supporting the SOLGASMIX system are discussed. An index listing the species in the curvefit database is included.

ABSTRACT

After a brief discussion of the theory of chemical equilibrium, the computer program SOLGASMIX, for calculating thermodynamic equilibria in complex chemical systems, is described. Modifications to SOLGASMIX which allow the program to access a database of thermochemical curvefits are discussed. Additional extensions to the SOLGASMIX program, including an interactive user interface, are introduced. Several SOLGASMIX applications are presented in detail, and the results of the program compared with those of other methods. Several additional programs, which allow the user to incorporate the curvefit database in other applications, are described. A number of input examples are given for the each of the various programs, and data punching guides are given where appropriate. The various operating systems supporting the SOLGASMIX system are discussed. An index listing the species in the curvefit database is included.

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ACKNOWLEDGMENTS

The author would like to express his appreciation to Dr. Richard Smith for his guidance in carrying out the work discussed in this paper, and for serving as advisor during the author's protracted tenure as a George F. Wisclicenus Undergraduate Assistant and Graduate Research Assistant.

INTRODUCTION

Among the tasks performed by an engineer involved in the analysis of chemical processes, the prediction of equilibrium states in chemical systems is one of the most important. The calculation of equilibrium composition is a necessary (and often initial) step towards the design of products and processes involving chemical reactions.

As defined by Smith and Missen[1], a system is at its equilibrium state if its composition is:

1. Independent of time.

2. Independent of the previous history of the system.

3. Resistant to fluctuations (within limits of magnitude but not of direction) of composition; that is, any such fluctuations are damped out.

Although any chemical system will tend to approach an equilibrium composition, an equilibrium model is not universally applicable to every reacting system. Since many chemical reactions proceed at extremely slow rates, there are a number of cases for which a true equilibrium composition is never obtained. Even those processes with very high rates may never approach equilibrium in a system with rapid externally applied compositional changes. Smith and Missen[2] give the following as indications of the applicability of an equilibrium analysis;

1. The equilibrium model may be useful when rates of change (reaction and mass transfer) are relatively rapid. This tends to be the case when temperature is relatively high, as in a rocket engine, or when catalytic activity is relatively high, as in the case of a sulfur dioxide converter. The inferences of analytical chemistry involving ionic species are also normally based on this model.

2. The equilibrium model may be useful in a positive sense as a reference state to which rate considerations are applied, as in the cases of maximum conversion in a chemical reactor, electromotive force (emf) of a chemical cell, and stagewise operations in separation processes.

3. The equilibrium model may be useful in a negative sense, such as in predicting too low a conversion or yield or in avoiding equilibrium with respect to certain undesired species.

4. The equilibrium model may be useful as a guide in choosing process conditions, including the evaluation of a catalyst, particularly in conjunction with the effects of changing conditions.

To which the author would like to add;

5. An equilibrium model may often be of more use when applied in a qualitative rather than a quantitative sense. In other words, even if the composition of a system is unlikely to approximate a calculated equilibrium (due to rate limitations, or other factors such as unfavorable catalysis), the generic effects of changing composition or ambient conditions can be approximated through equilibrium analysis.

6. An equilibrium model can be used quite effectively in an instructional setting to demonstrate the effects of ambient conditions or composition changes on chemical processes.

As the above discussion indicates, there are a number of cases in which the calculation of equilibria in chemical systems is of great importance to the thermodynamicist or engineer.

There are two general methods of calculating equilibria in complex systems. The oldest method involves the use of equilibrium constant expressions to develop a set of nonlinear algebraic equations which could be solved for the concentrations of the various species present in the equilibrium system. This approach to chemical equilibrium problems (known as the the "classical" method) is best suited for hand calculations of relatively simple equilibria. Brinkley[3,4] developed systematic calculational algorithms based on equilibrium constant expressions, for use on early computers and desk calculators. His extension of the classical method simplifies the calculational procedure by reducing the number of simultaneous equations that must be solved for complex chemical systems.

The second method of determining complex equilibria is that of White[5]. In this method, the equilibrium composition is determined by finding the conditions under which the total system free energy is minimized. The direct free energy minimization method is well suited for implementation on digital computers, as the iterative solution process requires no chemical knowledge or intuition. The apparent disparity between the classical and free energy minimization techniques was resolved by Zeleznik and Gordon[6], who demonstrated that the methods of Brinkley and White were functionally identical.

Since White first proposed the direct free energy minimization technique, digital computers have become widely available and many programs have been developed which implement variations of this method for equilibrium calculations. The remainder of this work will discuss one such program, and the modifications and enhancements made by the author.

SOLGASMIX

The SOLGASMIX computer program was first described in 1975 by Eriksson[7]. It is an outgrowth of earlier work in which the direct free energy minimization method was extended, first[8] to chemical systems containing gaseous mixtures and pure condensed (solid and/or liquid) species, and later[9], to systems containing condensed phase mixtures. Besmann[10] modified the SOLGASMIX code slightly by making use of the ideal gas law to allow the calculation of equilibria in systems with specified constant temperature and volume (T,V systems), as well as the constant pressure (T,P) systems for which the program was initially developed. Beahm[11], added code to allow SOLGASMIX to predict the circumstances under which additional species or mixtures would be present in the equilibrium mixture.

The total free energy of a chemical system can be expressed as;

$$G_s = \sum (n_i(\Delta G_i + RT \cdot \ln a_i)) \qquad [1]$$

Where:

G_s = Total system free energy

ΔG_i = Standard free energy of species i at temperature T

R = Gas constant

T = Absolute temperature

n_i = Molar amount of species i

a_i = Activity of species i

The total system free energy can conveniently be represented as the dimensionless quantity G_s/RT. In an ideal system containing a gaseous phase, one or more condensed mixtures, and one or more pure condensed species, this quantity can be represented by;

$$G_s/RT = \sum n_i \{ (\Delta G_i/RT) + \ln P + \ln(n_i/N) \}$$

$$+ \sum\sum n_i \{ (\Delta G_i/RT) + \ln(n_i/N) \} \qquad [2]$$

$$+ \sum n_i \{ \Delta G_i/RT \}$$

Where:

N = Total number of moles of all species in a mixture.

The first summation term applies to the gas phase. The second is a double summation over every species in each of the condensed phase mixtures. The last summation applies to pure condensed species, which can be considered to be single component mixtures. SOLGASMIX uses Lagrange's method of undetermined multipliers and a Taylor series expansion about an estimated compositional point in order to minimize equation [2]. The solution is further constrained by the fact that the molar amounts of each element in the equilibrium must be conserved. This can be expressed as;

$$\sum n_i A_{ij} = b_j \qquad [3]$$

Where;

A_{ij} = Coefficient on element j in formula
of species i

b_j = Moles of element j.

SOLGASMIX allows the user to take nonidealities into account by specifying activity coefficients (γ_i) for any species, which are multiplied by the n_i/N terms in the above summations.

The input to SOLGASMIX consists of a list of species which are to be considered as possible constituents of the equilibrium mixture. In addition to the atomic composition of each of these species, the user must provide the program with values for the standard Gibbs free energy of formation for each species, at every temperature for which an equilibrium solution is desired. Previous versions

of SOLGASMIX supported two methods of data entry. The first method required the user to provide the program with values for ΔH_i° (the standard free energy of formation for species i at 298 K), S_i° (the absolute entropy of species i at 298 K), and coefficients of a function for specific heat. The form of this specific heat curve was specified as follows;

$$C_{p,i}(T) = a + bT + cT^2 + d/T^2 + e/T^3 \qquad [4]$$

where T is the temperature in K and the values of the coefficients a...e were provided by the user for each species.

SOLGASMIX calculates the values of ΔG_i from the above using the relationship;

$$\Delta G_i = \Delta H_i - T\Delta S_i \qquad [5]$$

where;

$$\Delta H_i = \Delta H_i^\circ + \int C_{p,i}(T)\, dT$$
$$- \sum A_{ij} \int C_{p,j}(T)\, dT \qquad [6]$$

and;

$$\Delta S_i = S_i^\circ + \int C_{p,i}(T)/T\, dT$$
$$- \sum A_{ij} \left\{ S_j^\circ + \int C_{p,j}(T)/T\, dT \right\} \qquad [7]$$

Note that the integrals in the above expression are evaluated over the interval from 298 K to the temperature for which the value of ΔG is to be evaluated. The heat released by the reaction process leading to equilibrium is calculated from;

$$Q = \sum Y_i (\Delta H_i) - \sum X_i (\Delta H_i) \qquad [8]$$

Where Y_i represents moles of each product present at equilibrium, and X_i refers to the starting amounts of each reactant.

The second method available for providing thermochemical data to SOLGASMIX is to enter the coefficients of a curvefit for the value of $\Delta G(T)$ for each species in the equilibrium set of phases. The function has the form;

$$\Delta G(T) = a/T + b + cT + dT^2 + eT^3 + fT\ln(T) \qquad [9]$$

where the six coefficients a...f are provided as input to the program.

Extensive use of SOLGASMIX[12] demonstrated that most of the effort involved in compiling a data deck for use with the program was expended in finding or deriving accurate curvefits for either C_p or ΔG values for the various species possibly present in the equilibrium composition. While a number of sources of thermochemical data give coefficients of C_p functions in a format that is immediately useable by SOLGASMIX (for example, see Barin, Knacke[13]), the accuracy of these curvefits is often unknown. In addition, the requirement that C_p curvefits must be valid over the entire temperature range from 298 K to the desired equilibrium temperature limits the effectiveness of the first method of data entry. The usefulness of the second data entry option is limited by the lack of tabulated curvefits for ΔG functions, and also by the fact that if heat of reaction calculations are desired, it is necessary to specify both C_p and ΔG curvefit coefficients.

In order to enhance the performance of SOLGASMIX, an extensive library of curvefits of known accuracy was developed to interface with the program. This effort is discussed in subsequent sections.

THE JANAF CURVEFIT DATABASE

Among the most widely used sources of thermochemical data are the JANAF (Joint Army, Navy, Air Force) thermochemical tables[14]. Although originally developed for use in propulsion calculations, this document contains tabulated data for a variety of species applicable to many classes of chemical processes. As a source of data for SOLGASMIX, the JANAF tables offer numerous advantages. First, the tables are widely accepted throughout the various engineering communities as an accurate and reliable source of thermochemical data. Second, the fact that 1796 species are represented in the third edition (the latest release, as of this writing) makes the JANAF tables one of the most extensive compilations of data available. Finally, since the tables were originally created on a computer, it was possible for the author to obtain an advance release of the tables in a computer readable format.

The JANAF tables contain tabulated data for a number of thermochemical functions, including specific heat and Gibbs free energy values. Since C_p values are discontinuous at both first and second order phase transitions[15], it was recognized that a greater number of curvefits would be required to represent C_p functions than would be needed to predict ΔG values to similiar accuracy. Therefore, curves were fit to the ΔG values for each species in the JANAF tables. Curvefits were also developed for the enthalpy change;

$$H(T) - H(298) = \int C_p(T)dT$$

Thus, SOLGASMIX can predict heats of reaction by directly calculating the $\int C_p(T)dT$ terms which appear in equations [6] and [7]. Again, elimination of the need for specific heat functions enhances the accuracy of the results. The form of this second set of curvefits is;

$$H(T) - H(298) = a + bT + cT^2 + dT^3 + e/T + f/T^2 \qquad [10]$$

which was chosen by considering the effects of integrating a function in the form of equation [4].

The program FITTER6 was developed to read data directly from the JANAF tape as received from the National Bureau of Standards, and fit curves to the tabulated ΔG and H(T)-H(298) data for each of the species in the tables. FITTER6 calls the IMSL routines BECOVM and RLMUL to perform the actual multiple linear regression analysis[16]. The ΔG functions have the form of equation [9], with two extensions. First, in some cases, more than one curve was necessary to represent the Gibbs free energy function accurately. Therefore, a number of species have more than one set of coefficients in the database, along with a corresponding value for the temperature of transition between the two curves. Second, every element has, by definition, a null value for its Gibbs free energy of formation when in its reference state. In order to ensure that the curvefits to the ΔG functions accurately reflect this requirement, two additional variables are supplied in the database, reflecting the beginning and end, respectively, of a temperature range in which the Gibbs free energy of formation has a value of zero.

Since the H(T)-H(298) curvefits are discontinuous at first order phase transitions, and a number of species are tabulated for which there are two such transitions (usually at the liquification and vaporization points), up to three sets of curvefit coefficients are provided in the database, along with transition temperatures.

In order to provide an indication of the accuracy of the curvefits produced by FITTER6, a set of statistical parameters are provided in the database to represent the degree of fit for both the Gibbs free energy and enthalpy change functions. The statistical data reflecting the error in the

curvefits (the difference between the original tabulated data and the values obtained through use of the curves) includes the maximum, mean, and standard deviation of the percentage error, and the absolute value of the maximum error in kilojoules per mole. Table 1 summarizes the statistical data for the entire set of curvefits. Note that for most of the species for which curvefits were generated, the free energy curves yield results which lie within 2% of the tabulated values. Note also that a considerable number of both the ΔG and $H(T)$ - $H(298)$ curvefits have maximum percentage errors greater than 100%. In the large majority of these cases, the enormous percentage error is due to a very small tabulated value rather than to a large actual error. Most of the time, these errors are insignificant when compared to the magnitude of the other values involved in the equilibrium or heat of reaction calculations.

In order to allow the user to judge the acceptability of equilibrium results based on data from the JANAF curvefit database, a complete set of statistical data for each curvefit is included in the SOLGASMIX output. In addition, the maximum temperature for which data is tabulated in the JANAF tables is printed, along with the number of data points used for the curvefit. Caution is urged when using the curve fits to predict thermochemical properties at temperatures below 298 K or above the maximum tabulated value as reported by the program. While the curvefits provide for highly accurate interpolation of results between adjacent data points in the JANAF table, no guarantee can be made regarding the suitability of these curves for extrapolation. Figures 1 and 2 show the correlation between JANAF table data and typical curvefits for $H(T)$ - $H(298)$ and ΔG values, respectively.

The use of the curvefit database as a source of thermochemical data for SOLGASMIX is a third data entry option in the new version of SOLGASMIX. A

complete data punching guide for the program is included in Appendix A. Appendix B contains a number of short example data decks for the program, illustrating the features of each of the data entry options.

In order to use the database as a source of thermochemical data, the user must specify all species formulae according to the modified Hill indexing system[17], as used in the JANAF tables. Appendix C is an index listing every species available in the database, along with its correct Hill formula name. Appendix G presents a short discussion of the interactive utility program J-IND, which can be used to create a good portion of the input deck for a SOLGASMIX job. J-IND ensures that the correct Hill formula names are used for each species in the equilibrium system.

Although the JANAF curvefit database contains data for a large number of chemical species, many users will need access to data for species not included in the JANAF tables. The JFIT program is a modification of FITTER6 which allows each user to create an auxilliary database of curvefits for species not included in the JANAF tables. The thermochemical curvefits contained in this auxilliary database will then be accessed by SOLGASMIX as needed. Appendix D contains a data punching guide and an example data set for JFIT.

Although the curvefit database was originally created for use with SOLGASMIX, some users will find the data applicable to a number of other types of problems. For this reason, the subprograms JREAD, HFUN and GFUN were created to facilitate the use of curvefit data within application programs. JREAD returns the curvefit coefficients and statistical data for one or more species, while HFUN and GFUN use these coefficients to calculate values of $H(T)-H(298)$ and ΔG, respectively. Appendix E is a detailed guide to the use of these programs. Appendix F contains a listing for the short application program

JRACT, which calls JREAD, HFUN and GFUN in order to perform heat of reaction and free energy of reaction calculations for any chemical process.

Figure 3 is a diagrammatic representation of the entire SOLGASMIX system, showing the interrelationships between the various programs and data files discussed previously.

OTHER MODIFICATIONS TO SOLGASMIX

Although the most significant modifications to SOLGASMIX relate to the interface with the JANAF curvefit database, the author has made numerous other changes designed to enhance the usefulness of the program. With the exception of subroutines GASOL, ABER and XBER, major changes were made to each section of SOLGASMIX. Despite the scope of these extensions and modifications, every effort was made to maintain compatibility with data decks created for use with earlier versions of the program. The most obvious difference between earlier data formats (see Besmann[10]) is that all read statements in SOLGASMIX have been converted to list directed (free format) input. Experience has shown that this significantly reduces the tedium of creating a data deck for use with the program. As discussed in Appendix A, the free format input setup requires the user to enclose all character strings (i.e: the species names) in single quotes, and insert commas or spaces between successive data items on a single input line.

On machines which support interactive processing (see Appendix H for a discussion of the various operating systems supported by the latest version of SOLGASMIX), several subroutines have been added which comprise a "menu" of interactive features. The menu allows the user to change some of the parameters in the equilibrium system without creating an entirely new data deck. Using this feature, one can interactively change the ambient pressure or temperature conditions, the system volume, or the initial molar amounts of one or more species in the equilibrium set of phases. The author has found this facility to be extremely useful, particularly where the effects of subtle changes in system composition or ambient conditions are to be investigated. Another feature added to the latest version of the program allows SOLGASMIX to predict the adiabatic flame temperature of a system by iteratively solving for equilibrium at various

temperatures until the heat of reaction becomes negligible. The author has found this to be a significant enhancement of the program's capabilities, especially when combined with the other interactive processing options.

Other changes to the program have generally been minor in nature. The program output has been changed slightly to present additional useful data (Appendix B.2 is an example of a SOLGASMIX output listing). Several sections of code were added to avoid commonly occurring error messages. For example, in certain portions of subroutine GASOL, the mole fraction of a species may be calculated as an extremely small ($\simeq 10^{-80}$) value, which causes a run time error. To correct for this condition, the mole fraction is set equal to zero, which avoids the error. A summary of the number of errors corrected by this and similar "patches" is printed at the end of each run of the program.

TESTS OF PROGRAM ACCURACY

Since the latest version of SOLGASMIX contains extensive modifications to every portion of the program, a number of jobs were run in order to allow comparison between the equilibrium values predicted by the modified program and those arrived at using other methods. As an example, consider the production of lime from calcium carbonate (limestone). For this reaction;

$$CaCO_3 \text{ -------> } CaO + CO_2 \uparrow$$
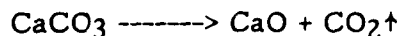
the equilibrium constant K_p is given by:

$$K_p = [CO_2][CaO]/[CaCO_3]$$

where the bracketed values represent the partial molar fractions of each constituent. Since it has been observed that the solid calcium carbonate and calcium oxide constituents are immiscible, K_p is numerically equal to the partial pressure of CO_2 (if an ideal gas assumption is employed). Since[18]:

$$\ln(K_p) = -\Delta G_{rxn}/(RT)$$

values of the partial pressure of CO_2 predicted by SOLGASMIX can be directly compared to theoretically predicted values for K_p. This comparison is shown graphically in Figure 4 over the temperature range from 500 - 1100 K (440 - 1520°F).

Since $CaCO_3$ is not included in the JANAF tables, it was necessary to provide SOLGASMIX with some means of calculating values for the Gibbs free energy of this species. One method would have been to use JFIT to add calcium carbonate to the auxilliary (user specified) database, as discussed in Appendix D. The second method is illustrated in the first sample data deck of Appendix B, and is the data setup used for the SOLGASMIX predictions here discussed. In this example, the curvefits for ΔG are specified as in equation [9]. Note that only two coefficients are given for each curvefit, which approximates the Gibbs free

energy function as a linear function of temperature. Even with this rather crude approach, the maximum difference between the theoretical value of K_p and the partial pressure of CO_2 predicted by SOLGASMIX is approximately 3%, as shown in Figure 4.

The second short example data deck in Appendix B is for the calculation of the equilibrium between water and its vapor. The results are compared with values from the literature in Figure 5. The maximum difference between the calculated and measured values of Figure 5 is under 3%, thus providing evidence of the usefulness of SOLGASMIX when applied to this multiphase equilibrium system. In this example, the JANAF curvefit database is used as a source of thermochemical data, so no coefficients for ΔG functions are included in the data deck. Note that the species "WATER(L)" is referenced in the program input, but is not included in the JANAF tables. In order to include this species in an equilibrium problem, the curvefit database must first be customized by the user with the JFIT program. The JFIT example included in Appendix D contains the necessary data to generate thermochemical curvefits for liquid water at low temperatures, as well as for several other species.

As a final test of the accuracy of the modified version of SOLGASMIX, the combustion of a hydroxyl amine monopropellant was analyzed using both SOLGASMIX and CEC76, a chemical equilibrium program produced by NASA[19]. CEC76 is widely used for gas phase combustion or detonation problems, but lacks the flexibility of SOLGASMIX when used for systems containing large amounts of condensed phase products. The products of the gas phase monopropellant combustion as predicted by both programs are compared in Table 2. The two sets of results are seen to agree to within 5%, with only minor discrepancies resulting from differences in the two calculational algorithms. The data deck used for SOLGASMIX is included as the third example in Appendix B.

LIMITATIONS ON THE USE OF SOLGASMIX

The examples discussed above all attest to the accuracy of SOLGASMIX calculations when compared with the results of other equilibrium programs and equilibria predicted by "classical" means. It is essential to note, however, that there is a large class of problems for which an equilibrium analysis is not a valid predictor of the actual composition of a chemical system. For this reason, extreme care must be taken before the results of any type of equilibrium study are utilized as the basis for the inclusion of a chemical process into an engineering system. A simplistic example of this is the nitrogen/hydrogen equilibrium given in the fifth example of Appendix B. SOLGASMIX predicts the formation of large amounts of ammonia. In the actual commercial production of ammonia, pressures an order of magnitude greater than the 10 atmospheres of example 5 are necessary, and a catalyst must be used to speed up the reaction to a level at which it becomes commercially feasible. In this example, the results of equilibrium predictions are not consistent with actual chemical phenomena. Some instances in which an equilibrium analysis of a reacting system is likely to disagree strongly with observed results include:

1. Cases in which a reaction has a very slow rate. It is necessary in interpreting the results of an equilibrium analysis to first check for any product species which is known to form very slowly.

2. Processes with high activation energies.

3. Chemical systems which never reach equilibrium without catalysis. Catalysts do not change the equilibrium state of a system: they merely change the rate of a system's progress toward this state. Some reactions are unfavorably autocatalytic, and thus may never reach equilibrium.

4. Processes dependent upon the mixing of chemical species may proceed only to a limited extent. For example, the oxide film which quickly forms on a fresh aluminum surface generally prevents further corrosion of the bulk of the metal, although an equilibrium calculation would indicate complete conversion to Al_2O_3.

An important consideration regarding the applicability of SOLGASMIX to specific chemical systems arises from the form of equation [2]. This equation, which gives the total Gibbs free energy of a system, involves several implicit assumptions. All mixtures are, by default, assumed to be ideal. In systems for which there are nonidealities present, activity coefficients must be specified (by modifying subroutine FACTOR) in order for the output to agree with observed phenomena. Unfortunately, the availability of activity coefficients for a system usually implies considerable previous empirical work, in which case SOLGASMIX results are less likely to be of critical importance. For this reason, most users will find themselves forced to assume ideality for each mixture in a problem.

A related assumption, also implicit in equation [2], is that the ideal gas law is used to predict values of Gibbs free energy for pressures other than atmospheric. At conditions near the critical point for a gas, this approximation can be very inaccurate. For this reason, when using SOLGASMIX for gas phase equilibria under ambient conditions of high pressure and low temperature, the user is well advised to consider the effects of nonideal gas behavior when analyzing the program output.

One final caution regarding the accuracy of SOLGASMIX equilibrium predictions refers not to a shortcoming in the program itself, but in the way some users approach an equilibrium calculation. Because only species specified by the user are tested for inclusion in the equilibrium mixture, it is possible to overconstrain a problem by specifying too few species. In other words, if a species which would otherwise comprise a significant portion of the equilibrium mixture is left out of a SOLGASMIX input data deck, the calculated equilibrium will be completely erroneous. It is therefore necessary to include every species in the data deck which might conceivably be included in the products of an actual

reaction. The author's approach has been to scan the index to the JANAF tables (see Appendix C) and include all species which are comprised exclusively of the set of elements which make up the input to the program. In addition, since the JANAF tables are by no means a complete compilation of all chemical species, several other sources of thermochemical data are perused to spot any species not included in the curvefit database; these species are then added to the auxilliary database using the JFIT program.

In order to reduce the tedium of poring over the index of species, the author has created the J-IND general purpose index program for use with the JANAF tables. As discussed in Appendix G, this program can do the bulk of the work needed to create a data deck for use with SOLGASMIX.

CONCLUSIONS

For the engineer or physical chemist, few analyses are as important as the prediction of chemical equilibrium. For complex multiphase chemical systems, however, this calculation can be extremely tedious. The use of computer algorithms based on the minimization of the total system free energy allows one to calculate the equilibrium state of extremely complex chemical systems, which would be essentially impossible to analyze by hand.

The program SOLGASMIX has been demonstrated to successfully implement a free energy minimization algorithm, and has been used extensively to predict the products of numerous chemical interactions. With the addition of an interface to the JANAF curvefit database, SOLGASMIX has become a very powerful and easily applied tool for the thermochemical analysis of reacting systems.

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## TABLE 1: DISTRIBUTION OF ERROR IN CURVEFITS.

NUMBER OF SPECIES IN EACH ERROR BAND.		
PERCENT ERROR	H(T)-H(298)	$\Delta G°$
UNDER 2 %	1595	1449
2% - 10%	113	123
10% - 20%	21	32
20% - 30%	12	16
30% - 40%	9	20
40% - 50%	2	14
50% - 60%	6	10
60% - 70%	8	8
70% - 80%	2	4
80% - 90%	2	3
90% - 100%	3	5
OVER 100%*	23	112
TOTAL	1796	1796
AVERAGE % ERROR*	1.98	2.95

* As discussed in the text, the large percentage errors (100% or larger) which occur in a number of the curvefits do not, in general, represent large numerical errors. For this reason, species with curvefit errors larger than 100% were ignored in calculating the average percentage errors given above.

TABLE 2: COMPARISON OF CEC76 AND SOLGASMIX PREDICTIONS OF HYDROXYL AMINE MONOPROPELLANT COMBUSTION.

REACTANTS (WEIGHT PERCENTAGES)	
$N_2H_4O_4$	61.0 %
H_2O	20.0 %
$C_6H_{16}N_2O_6$	19.0 %

PREDICTED COMBUSTION PRODUCTS (MOLE FRACTIONS) AT 1600 F (1144 K) AND 200 ATM. PRESSURE		
	SOLGASMIX	CEC76
CO_2	12.303 %	12.302 %
H_2O	70.925 %	70.912 %
N_2	16.587 %	16.594 %
O_2	0.183 %	0.191 %
NO	$5.94*10^{-4}$ %	$6.07*10^{-4}$ %

FIG 1: EXAMPLE OF H(T)—H(298) CURVEFIT

TEMPERATURE (K)

—— CURVEFIT   * * * JANAF

DATA SHOWN IS FOR SODIUM: NA1(REF)

H(T)—H(298) : KILOJOULES PER MOLE
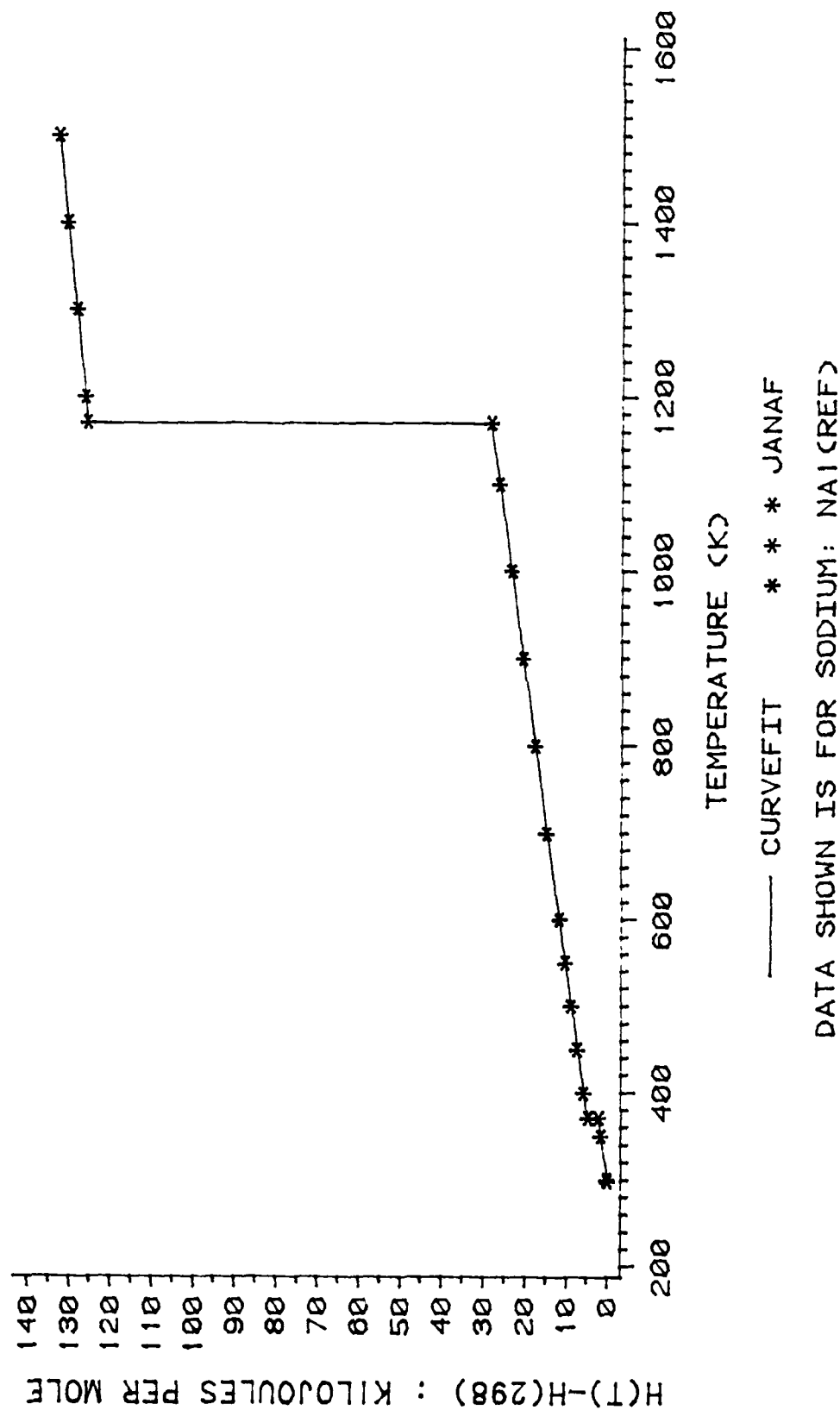
FIG 2: EXAMPLE OF GIBBS FREE ENERGY CURVEFIT

FREE ENERGY : KILOJOULES PER MOLE

TEMPERATURE (K)

—— CURVEFIT   * * * JANAF

DATA SHOWN IS FOR IRON: FE1(CR)
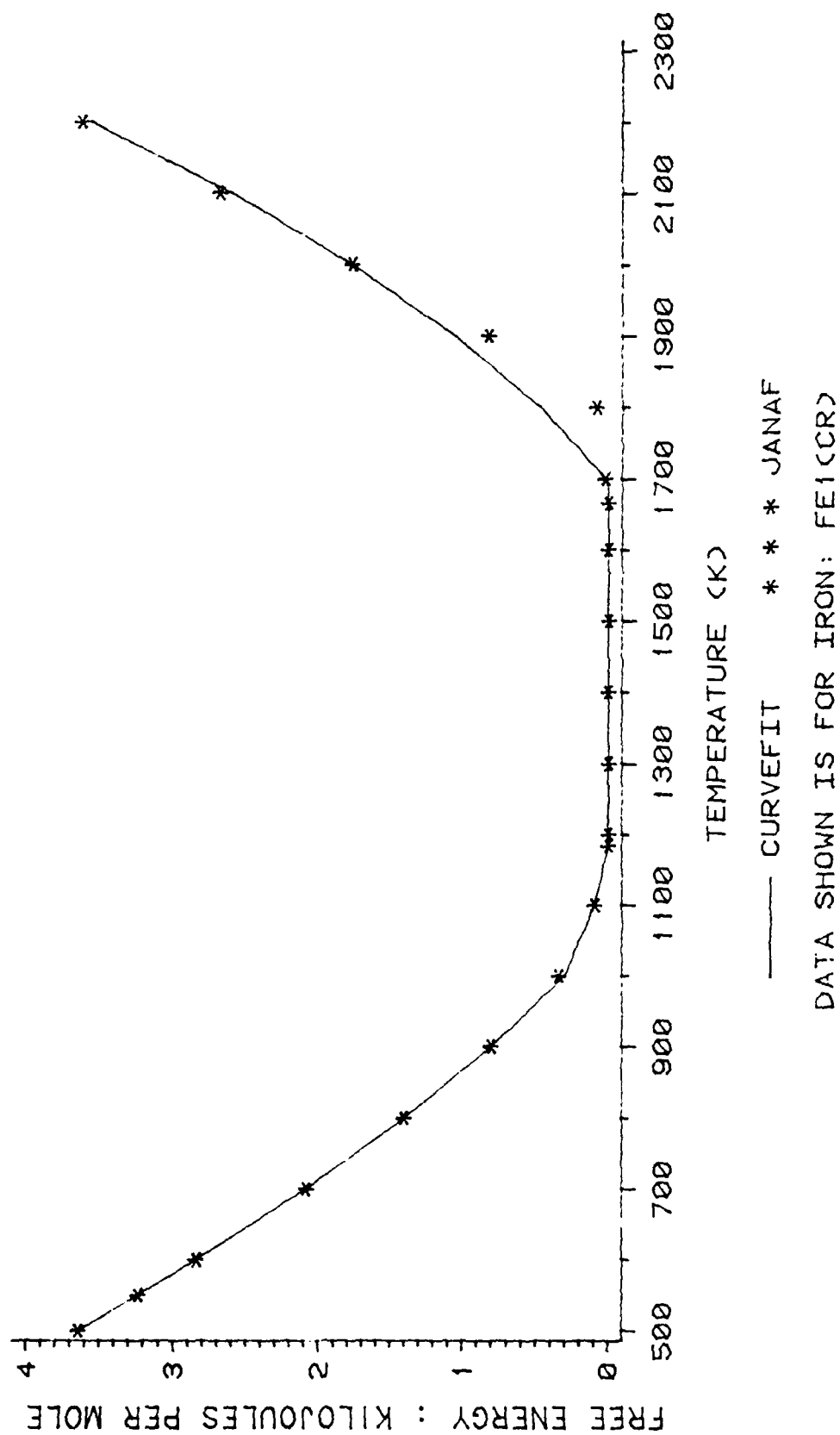
FIG. 3: FLOWCHART OF SOLGASMIX SYSTEM
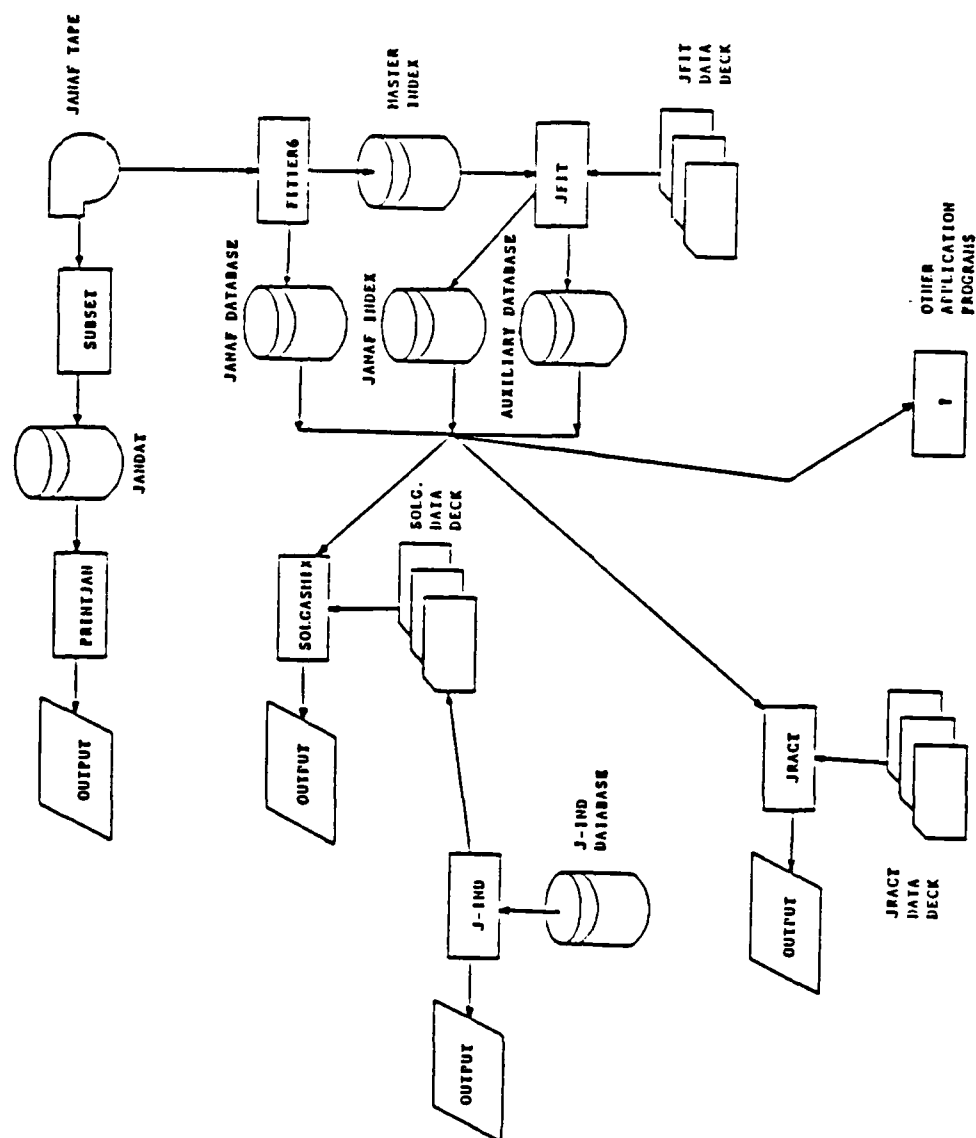
FIG 4: CaCO3 ———> CaO + CO2
LOG OF EQUILIBRIUM CONSTANT VS. TEMPERATURE
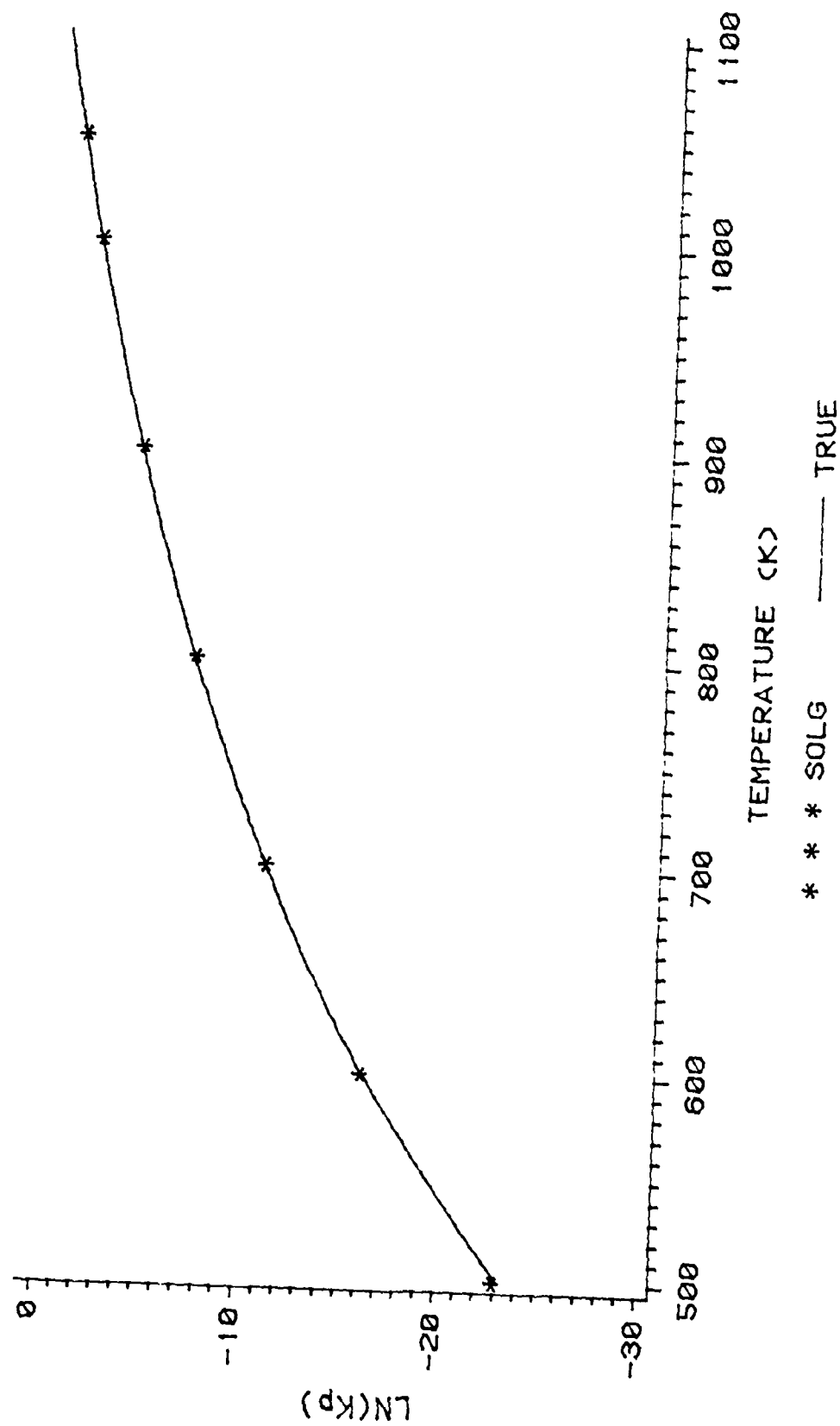
FIG 5: WATER VAPOR PRESSURE

PRESSURE (ATM)

TEMPERATURE (C)

* * * SOLG

——— TRUE
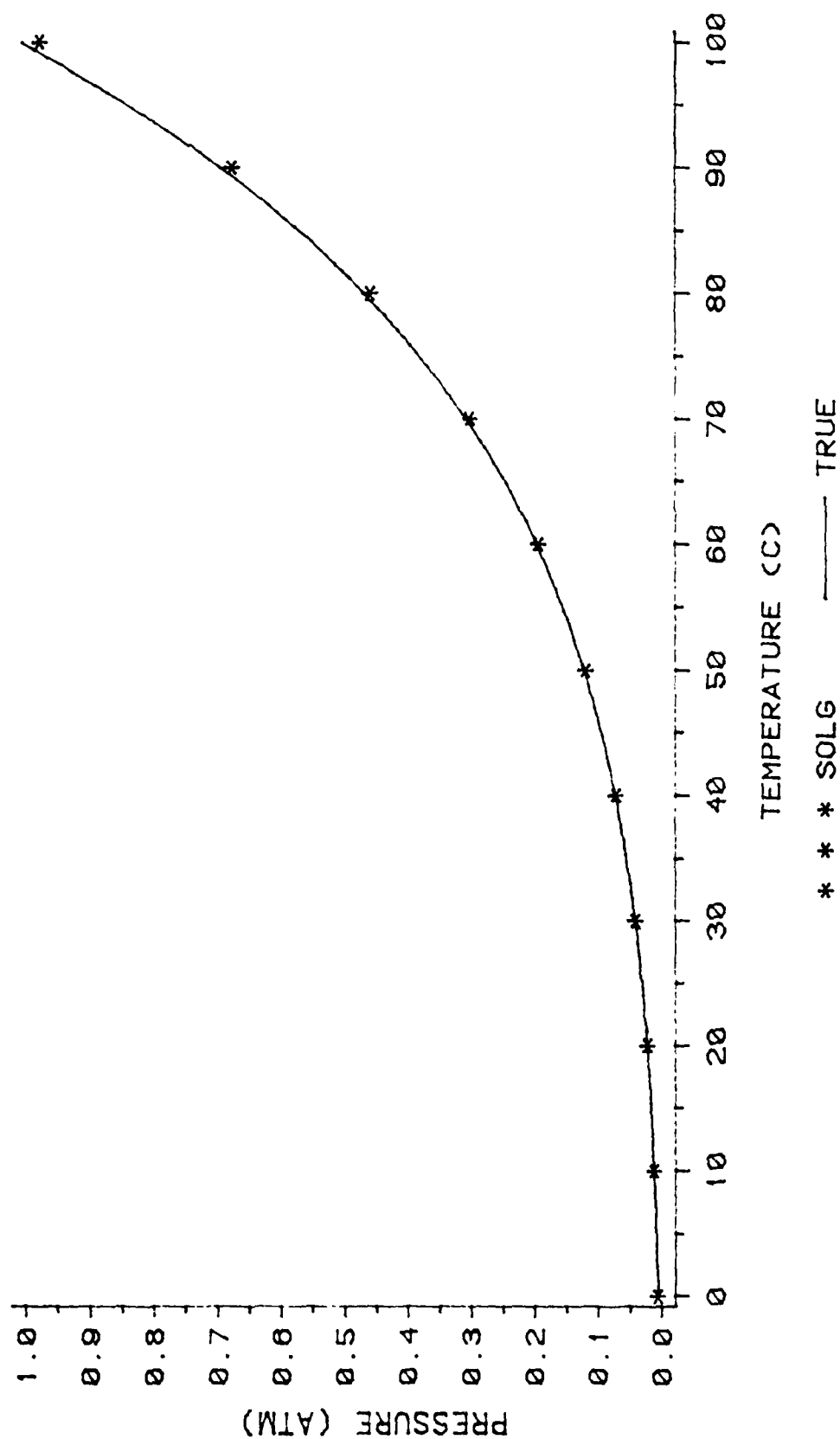
APPENDIX A: GUIDE TO THE USE OF SOLGASMIX.

The recent modifications to SOLGASMIX have all been intended to make the program easier to use, while simultaneously increasing the accuracy of the program output. In order to make the latest version of the program as useful as possible, the capacity to run data decks created for earlier versions of the program has been retained. For example, the sample card deck of Appendix H (set up for use with the batch version of SOLGASMIX on the PSU MVS system) is the same as that given by Besmann (10). The only changes to the card deck are the fact that the species names are enclosed in single quotes, and unformatted input is used, requiring spaces or commas between intervening data entries on the same line (but freeing the user from the requirement of adhering to rigid data formats).

Unfortunately, since SOLGASMIX has been modified so many times over the course of the last decade by numerous users, the data punching guide is likely to be somewhat confusing to the beginning user. For example, if heat of reaction calculations are desired, the initial composition of the (unreacted) mixture is specified by entering the amounts of each species in the system. However, if no heat calculations are to be performed, the user must specify the amounts of each constituent element, regardless of which species are considered as the starting point of the reaction. Because of the confusion so often caused by the disparities between the numerous input options, two punching guides are included below. The first is the complete guide to SOLGASMIX input, including all the options available in the latest version. The second data guide is a truncated setup, showing the simplest form of input to the program. The author has found most of various data entry options to be superfluous to everyday use of the program, and generally follows the data format of this simpler punching guide. It is recommended that the user follow the short form of the data guide for the most part, while becoming familiar with all of the capabilities of the program as documented in the longer data punching guide. Following the punching guides is a discussion of some commonly occurring error conditions and ways to rectify them.

Note that all temperatures entered as data to SOLGASMIX and the other programs discussed in this work are in K, while pressures are given in atmospheres.

A.1: DATA PUNCHING GUIDE FOR ARL/PSU SOLGASMIX

Note: highlighted sections have been added to SOLGASMIX
At the Pennsylvania State University.

CARD   VARIABLE NAME

1.   TITLE   Anything punched on this line will
                         be repeated at the top of each
                         output page.

2.   L   The number of elements in the
                         chemical system $(L \leq 10)$.

          MP   The total number of gaseous, liquid
                         and solid mixtures $(MP \leq 20)$.

          MR   The total number of condensed
                         phases of invariant stoichiometry,
                         not part of any of the MP mixtures.

          ML(1)   The number of species in mixture 1.
                         Mixture 1 is always the gas phase.

          ML(2)   The number of species in mixture 2.
          .
          .

          ML(MP)   The number of species in the last
                         mixture.

3.   EL(1)   The symbol for the first element.
                         **The elemental symbols must be
                         enclosed in single quotes.**

          EL(2)   The symbol for the second element.
          .
          .

          EL(L)   The symbol for the last element.

   Note: The total number of species is given as the
         variable MS. $MS = ML(1) + ML(2)$
         $+ \ldots + ML(MP) + MR$. MS must be less
         than or equal to 125.

4.   TEXT(I)   The name for species number I.
                         **For use with the JANAF curvefit
                         database, TEXT may be up to 29
                         characters long and must exactly
                         match the species names given in
                         Appendix C. Note that the names
                         will be truncated to 8 characters
                         for output.**

A(I,1)   The coefficient on the elemental
                symbol of element 1 in species I.

A(I,2)   The coefficient on the elemental
                symbol of element 2 in species I.
.
.
A(I,L)   The coefficient on the elemental
                symbol of element L in species I.

Note: There is one card #4 for each species for a total
      MS cards. The species order should be defined as
      follows: Species in mixture 1 (gas phase),
      species in mixture 2, and so on, followed by
      the condensed phases. Note that within each
      mixture, putting the species that are most
      likely to be present in the equilibrium mixture
      first will result in faster execution time.
      Note also that if the equilibrium activity
      for a species will be specified, this species
      must be regarded as an element in its chosen
      reference state.

5.   IEL(1)   The number of the species for
                          element number 1 in its chosen
                          reference state.

          IEL(2)   The number of the species for
                          element number 2 in its chosen
                          reference state.
          .
          .
          IEL(L)   The number of the species for the
                          last element in its chosen
                          reference state.

6.   KVAL2   Main Control card. Indicates which
                          program options are desired.

=1: No heat of reaction calculations performed. Values
    of the coefficients of the function $\Delta G(T)$
    as thermodynamic input.

=2: No heat of reaction calculations performed. Values
    of $\Delta H°$, $S°$, and coefficients of the function
    $C_p(T)$ as thermodynamic input.

=3: Heat calculations performed. Coefficients of the
    functions $\Delta G(T)$ and $C_p(T)$, and values of
    $\Delta H°$ and $S°$ as thermodynamic data.

=4: Heat of reaction calculations performed. Values
    of $\Delta H°$, $S°$, and coefficients of the function
    $C_p(T)$ as thermodynamic input.

=5: Heat calculations performed. Thermodynamic data read from the JANAF curvefit database. See below for punching guide for this value of KVAL2 only.

=6: No heat calculations. Thermodynamic data read from JANAF curvefit database (and/or user defined extensions to the database).

> Note: If KVAL2 is entered as -2, -4, or -5, heat calculations will be performed (the absolute value of KVAL2 is taken as the proper control value), but the values of thermochemical properties as calculated by the program will not be printed.
>
> This can result in a great savings in the amount of output generated by the program.

CONTINUE WITH CARD NUMBER 9 IF KVAL2 = 2, 4, 5, OR 6.

7.   MGT   The number of coefficients (X) in the expression $\Delta G(T) = X_1/T + X_2 + X_3T + X_4T^2 + X_5T^3 + X_6TLn(T)$ which are to be used to calculate ΔG.

          IGT(1)   The number "i" for one of the X_i

          IGT(2)   The number "i" for another X_i
            •
            •
          IGT(MGT)   The number of the last coefficient.

8.   GE(I,1,1)   The value of the coefficient IGT(1) for species number 1.

          GE(I,1,2)   The value of the coefficient IGT(2) for species number 1.
            •
            •
          GE(I,1,MGT)   The value of the last coefficient (IGT(MGT)) used for calculating ΔG for species number I.

     Note: There is one card #8 per species in the same order used for card #4, for a total of MS cards. The value of $\Delta G(T)$ has units of Joule/Mole

9.   T   The value of the equilibrium temperature (K).

CONTINUE WITH CARD NUMBER 16 IF KVAL2 = 1 OR 6, OR
IF KVAL1 < 9. KVAL1 = 9 AT START OF PROGRAM.
CONTINUE WITH CARD NUMBER 13 IF KVAL2 = 5.

10.   HF(I) ΔH° (the standard heat of formation) of species number I.

          S(I) S° (absolute entropy) for species number I.

Note: The value of HF in units of Joule/Mole. The value of S is in Joule/Mole/K. There is one card per species, in same order as card 4.

11.   NOM(1)   The number of $C_p(T)$ functions for species number 1.

          NOM(2)   The number of $C_p(T)$ functions for species number 2.

          NOM(MS)   The number of $C_p(T)$ functions for the last species.

12   C(I,J,1)   The value of "a" in the expression $C_p(T) = a + bT + cT^2 + d/T^2 + e/T^3$ for the J'th C_p function for species number I.

          C(I,J,2)   The value of b for the J'th C_p function for species number I.

          C(I,J,5)   The value of e for the J'th C_p function for species number I.

          TOM(I,J)   The temperature (K) of the transition from C_p expression J to C_p expression J+1 for species number I. This value only has significance if NOM(I) is greater than J.

          HOM(I,J)   The enthalpy of transition (J/Mole) for the above transition. Has significance if NOM(I) is greater than J.

Note: There are NOM(I) cards per species, for a total of MS species. The order of species is as entered in card #4. The value of C_p has units of J/Mole/K.

CONTINUE WITH CARD 16 IF KVAL2=2

13.   MIN   The number of species present in the raw material before reaction (non equilibrium mixture).

        IIN(1)   The species number for one of these species.

        IIN(2)   The species number for another one of these species.
        .
        .

        IIN(MIN)   The species number for the last species initially present in the unreacted mixture.

14.   T0   The temperature of the raw material before reaction (K).

CONTINUE WITH CARD 16

15.   PTOT   The total pressure on the equilibrium mixture (atmospheres), or the system volume (liters). For pressure, PTOT is positive. For volume, punch with a "-" sign.

16.   KVAL1   Second control card. Controls program flow.

=1: A starting estimate for the equilibrium composition will be entered by the user. Continue with cards 17, 18, 19, 20, and (*) 16.

=2: A starting estimate for the equilibrium composition will be generated by the program. Continue with cards 17, 18, 19, and (*) 16.

=3: The values of NPKT, KH, and B to be used in the next group of calculations are different from those used in the previous group. Continue with cards 17, 18, 19, and (*) 16.

=4: The values of NPKT and KH to be used in the next group are equal to those used in the previous group, but the values of B are different. Continue with cards 19 and (*) 16.

=5: The values of NPKT, KH, and B to be used in the next group are the same as those used in the previous group. Continue with card (*) 16.

=6: The value of the reaction temperature will be changed. Continue with cards 9 and 16.

=7: The calculations are to be performed for a constant volume system, or the equilibrium pressure is different from 1 atmosphere. Continue with cards 15 and 16.

=8: New values of GE are to be entered. Continue with card 8.

=9: At a transfer to a new system. Continue with card 1.

=10: Terminates program execution.

=12: Displays a menu, allowing the user to interactively change the temperature, volume, pressure, or composition of the problem. In noninteractive versions of the program, program execution is terminated.

Note: The term "group" refers to a series of equilibrium calculations performed on a system at the same temperature and pressure. Each group of calculations has one or more "points." The composition of the initial mixture varies between points in the group, although the ambient conditions stay the same.

The only values of KVAL1 that are useful for the first group are 1, 2, or 7. Each of the other possible values for KVAL1 represents a decision which apply to the second and subsequent groups: for example, a second group to be run at a different temperature or pressure.

Equilibria will be calculated by SOLGASMIX at places indicated by an asterisk (*) in the above discussion.

17.	NPKT	The number of points in the group (NPKT$\leq$99).
18.	KH(1)	Describes the way in which the total amount or log(a) (a = the equilibrium activity), of element number 1 or species number IIN(1) varies between adjacent points in the group.
	KH(2)	Describes the way in which the total amount of element number 2 or species number IIN(2) varies between adjacent points in the

group.
.
.

KH(MIN)   Describes the way in which the
                 amount of the last element or
                 of species number IIN(MIN) varies
                 between adjacent points in the
                 group.

KH=1: Molar amount varies irregularly between points.
KH=2: Molar amount is constant over all points.
KH=3: Molar amount varies by a constant increment.

KH=4: Log(a) varies irregularly.
KH=5: Log(a) is constant.
KH=6: Log(a) varies by a constant increment.

Note: There are MIN values on card #18. If KVAL2 = 1,
      2, or 6 (no heat calculations performed),
      MIN is set equal to L, and the values on cards
      #18 and #19 correspond to the initial amounts of
      each constituent element. If KVAL2 = 3, 4, or
      5, the values on cards #18 and #19 each
      corresponding to one of the species which is
      initially present in the mixture before
      reaction.

      USE CARD 19A IF KH = 1 OR 4 (IRREGULAR),
      USE CARD 19B IF KH = 2 OR 5 (CONSTANT),
      USE CARD 19C IF KH = 3 OR 6 (INCREMENTAL).

19A.   B(J,1)   Moles or Log(a) for element number
                        J or species number IIN(J) at the
                        first point in the group.

          B(J,2)   Moles or Log(a) for element number
                        J or species IIN(J) at the second
                        point in the group.
          .
          .
          B(J,NPKT)   Moles or Log(a) for element number
                        J or species IIN(J) at the last
                        point in the group.

19B.   B(J,1)   Moles or Log(a) for element number
                        J or species IIN(J), which is
                        constant over all points in
                        the group.

19C.   B(J,1)   Moles or Log(a) for element number
                        J or species IIN(J) at the first
                        point in the group.

	STEP	The constant increment in the amount or log(a) of element J or species IIN(J) between points in the group.

Note: There are MIN cards #19.

20.	Y(1)	An initial estimate for the equilibrium amount of species 1 (in moles).
	Y(2)	An initial estimate for the equilibrium amount of species 2 (in moles).
	•	
	•	
	Y(MS)	An initial estimate for the equilibrium amount of the last species.

A.2: SHORT FORM OF DATA PUNCHING GUIDE

The shortened data deck, below, presents a simplified method for setting up the input to SOLGASMIX. It uses KVAL2=5; which causes the program to read thermochemical data from the JANAF curvefit database, and indicates that heat of reaction calculations are desired. The data deck setup as discussed below is a convenient starting point for building more powerful decks to make use of some of the advanced features of the program. Example #8 in Appendix B is set up in this fashion; the output from this example is included as Appendix B.2. Example #2 is similarly constructed, except that KVAL1 options are used to tell SOLGASMIX to automatically calculate equilibria at a number of temperatures (instead of forcing the user to go through the menu). Example #6 is set up in a similiar fashion, except that the starting estimates for the equilibrium composition are generated by the program instead of being entered manually.

CARD	VARIABLE NAME	
1.	TITLE	Anything punched on this line will be repeated at the top of each output page.
2.	L	The number of elements in the chemical system ($L \leq 10$).
	MP	The total number of gaseous, liquid and solid mixtures ($MP \leq 20$).
	MR	The total number of condensed phases of invariant stoichiometry, not part of any of the MP mixtures.
	ML(1)	The number of species in mixture 1. Mixture 1 is always the gas phase.
	ML(2) $\bullet$ $\bullet$	The number of species in mixture 2.
	ML(MP)	The number of species in the last mixture.
3.	EL(1)	The symbol for the first element. The elemental symbols must be enclosed in single quotes.
	EL(2) $\bullet$ $\bullet$	The symbol for the second element.
	EL(L)	The symbol for the last element.
4.	TEXT(I)	The name for species number I. For use with the JANAF curvefit database, TEXT may be up to 23 characters long and must exactly

match the species names given in Appendix C. Note that the names will be truncated to 8 characters for output.

	$A(I,1)$	The coefficient on the elemental symbol of element 1 in species I.
	$A(I,2)$	The coefficient on the elemental symbol of element 2 in species I.
	.	
	.	
	$A(I,L)$	The coefficient on the elemental symbol of element L in species I.
5.	$IEL(1)$	The number of the species for element number 1 in its chosen reference state.
	$IEL(2)$	The number of the species for element number 2 in its chosen reference state.
	.	
	.	
	$IEL(L)$	The number of the species for the last element in its chosen reference state.
6.	KVAL2	The integer value '5' or '-5'.
9.	T	The value of the equilibrium temperature (K).
13.	MIN	The number of species present in the raw material before reaction (non equilibrium mixture).
	$IIN(1)$	The species number for one of these species.
	$IIN(2)$	The species number for another one of these species.
	.	
	.	
	$IIN(MIN)$	The species number for the last species initially present in the unreacted mixture.
14.	T0	The temperature of the raw material before reaction (K).
16.	KVAL1	The integer number '1'

17.	NPKT	The integer number '1'
18.	KH(1..MIN)	On this line, enter an integer '2' for each of the MIN species in the unreacted mixture. Separate the values with spaces or commas.
19	B(J,1) . . B(MIN,1)	Moles of species IIN(1). Moles of species IIN(MIN).

Note: There are MIN cards #19, one for each species which is specified as being present in the raw material (nonequilibrium system).

20.	Y(1) . . Y(MS)	An initial estimate for the equilibrium amount of species 1 (in moles). An initial estimate for the equilibrium amount of the last species.
16.	KVAL1	The second KVAL1 control card. Usually, this is 10 or 12. See long version of data punching guide for all options.

A.3: COMMONLY OCCURRING RUN- TIME PROBLEMS.

As discussed in the text, considerable effort was expended to make the latest version of SOLGASMIX as robust as possible. A number of program segments were added to check for commonly occurring run time errors and automatically correct for them. This effort has largely been successful, to the extent that essentially all of the conditions that could potentially cause problems during program execution have been corrected for.

Nonetheless, there are still several situations in which SOLGASMIX arrives at an erroneous answer to an equilibrium problem, despite proper program execution. In some cases, the equilibrium results returned by the program will clearly be in error. This condition occurs when the program finds a local minimum in the total free energy function of a system, and is evidenced by the complete absence of one or more mixtures from the equilibrium set of phases. For example, SOLGASMIX might return an equilibrium in which all of the products are in the gas phase, even at temperatures well below the normal vaporization temperatures of the products. Fortunately, this problem is easily rectified when it occurs, as discussed below.

Another case in which SOLGASMIX does not find a proper equilibrium condition is the case in which the total free energy of a system fails to converge quickly on a minimum value. In this case, the program prints the message "THE EQUILIBRIUM CONDITION HAS NOT BEEN OBTAINED."

The solutions to both of the above problems are similar. In the first instance, SOLGASMIX must be forced to find the true minimum of the free energy function, instead of the minima which neglects one or more of the condensed species. In the second instance, either better initial guesses must be provided, or conditions must be set up under which the equilibrium is easier for the program to find. The author has found the following to be convenient ways of forcing the program to find the correct minimum for the system free energy.

1. In some cases, SOLGASMIX will fail to find an equilibrium the first time a problem is run, but will arrive at the solution on the second try. This can be accomplished by use of the interactive menu. Choosing the "GO WITH NEW SYSTEM" option from the menu without changing any of the ambient conditions or the initial composition of the system has the effect of letting SOLGASMIX "pick up where it left off." The composition arrived at in the last iteration will be the new starting point for the second series of iterations.

2. If initial estimates for the equilibrium composition have been specified, an attempt to improve the accuracy of these "guesstimates" should be made. If the program has been instructed to generate starting estimates (KVAL1=2), the data deck should be changed so that user supplied estimates be utilized.

3. In some instances, it is necessary to change the initial amounts of one or more species in the equilibrium. This is especially true for problems in which the set of initial molar amounts in a system corresponds to a stoichiometric case. The addition of a minute amount of one or more of the reactants may move the equilibrium in a direction to which the iterative solution can converge.

4.   In many cases the program will not converge to a solution at a given temperature/pressure (T,P) point, but will find a valid solution at different ambient conditions. In this case, one can start from conditions under which an equilibrium is calculated, and "sneak up" on the desired solution by varying the ambient conditions. In this case, the valid solution arrived at for one set of conditions will serve as the initial estimate for the next (T,P) point.

The above solutions can most readily be implemented through the menu, which is reached by specifying a value of 12 for KVAL1. This is one of the most useful aspects of the versions of the program which run on systems supporting interactive processing. A somewhat more complex fix which is occasionally necessary is described below:

5.   If SOLGASMIX returns a result in which a mixture appears to have been erroneously deleted from the equilibrium set of phases, the program must be forced to include that mixture in the calculated equilbrium. To do this, it may be convenient to add an inert species to the mixture in question. For example, the addition of a noble gas such as argon is sometimes necessary for problems in which almost all of the products are in the condensed phase. Likewise, adding an element to the problem which is present in only one species in the data set will force the inclusion of the mixture containing the reference state of that element. The technique most often used by the author is to add traces of two imaginary species to his data deck. The species "YOUCANTGETTIUM" and "UNOBTAINIUM" are entered into the auxilliary (user specified) database with the JFIT program. These species are specified with a zero value for ΔG at all temperatures, with no enthalpy change upon heating. Thus, neither the heat of reaction nor the equilibrium composition of the mixture is sensibly changed by the addition of these species, providing that the molar amounts of these species are small. The ninth example in Appendix B illustrates the use of these species as trace elements. This example deck causes SOLGASMIX to calculate three different equilibria. In the first, the existence of the liquid mixture is ignored, and erroneous results are obtained. For the second equilibria, some "**(CR)" is added to the second mixture. This has the effect of causing the program to find yet another invalid equilibrium condition, in which the gas phase is ignored. Finally, correct results are obtained when some "*(G)" is added to the gaseous phase, forcing the inclusion of this mixture into the set of phases. The sample data deck for JFIT (see Appendix D) causes the JFIT program to add *(G) and **(CR), along with several other species, to the auxilliary database.

APPENDIX B: EXAMPLES OF SOLGASMIX DATA DECKS AND OUTPUT LISTINGS.

EXAMPLE 1: This is the input deck for the $CaCO_3$ decomposition discussed in the text. Note that the coefficients of the Gibbs free energy curve are included in the data deck itself, instead of being read from the JANAF curvefit database.

```
EXAMPLE 1: CACO3 DECOMPOSITION
4 1 4 3
                  'AR'      'C'      'CA'      'O'
'ARGON'           1.       0.       0.       0.
'CO2'             0.       1.       0.       2.
'O2'              0.       0.       0.       2.
'C'               0.       1.       0.       0.
'CA'              0.       0.       1.       0.
'CAO'             0.       0.       1.       1.
'CACO3'           0.       1.       1.       3.
1 4 5 3
1
2 2 3
0.0    0.0
-394550.    -1.2907
0.0    0.0
0.0    0.0
0.0    0.0
-635019.    104.529
-1201470.   256.08
500.
1
1
2 2 2 2
0.01
1.0
1.0
3.0
0.01  0.001  0.0    0.0    0.0    0.001 0.999
12
```

EXAMPLE 2: This is the input deck to predict the
equilibrium between liquid water and water
vapor. Note that the species "WATER(L)"
is a user defined extension to the curvefit
database, and as such requires the JFIT
program to be run first (see Appendix D).

```
EXAMPLE 2: VAPOR PRESSURE OF WATER
2,2,0,3,1
'H' 'O'
'H2(REF)'     2.0    0.0
'O2(REF)'     0.0    2.0
'H2O1(G)'     2.0    1.0
'WATER(L)'    2.0    1.0
1,2
-5
273.15
2,2,4
273.15
1
1
2 2
1.0
10000.0
0.00  1.00  0.00   10000.0
6
283.15
5
6
293.15
5
6
303.15
5
6
313.15
5
6
323.15
5
6
333.15
5
6
343.15
5
6
353.15
5
6
363.15
5
6
```

373.15
5
10

EXAMPLE 3: The example below predicts the products
of NOSET-1845 monopropellant combustion.
The JANAF curvefit database is used for
thermochemical data, but no heat calculations
are performed.

EXAMPLE 3: CARBON/HYDROGEN/OXYGEN/NITROGEN EQUILIBRIUM
4,1,1,53

		'C '	'H '	'O '	'N '
'N2(REF)	'	.00	.00	.00	2.00
'H2(REF)	'	.00	2.00	.00	.00
'O2(REF)	'	.00	.00	2.00	.00
'C3O2(G)	'	3.00	.00	2.00	.00
'C2O1(G)	'	2.00	.00	1.00	.00
'C3(G)	'	3.00	.00	.00	.00
'C2N1(G)	'	2.00	.00	.00	1.00
'C4N2(G)	'	4.00	.00	.00	2.00
'C2N2(G)	'	2.00	.00	.00	2.00
'N2O1(G)	'	.00	.00	1.00	2.00
'C2H4(G)	'	2.00	4.00	.00	.00
'C2(G)	'	2.00	.00	.00	.00
'H1N1O1(G)	'	.00	1.00	1.00	1.00
'C2H1(G)	'	2.00	1.00	.00	.00
'C1H1N1(G)	'	1.00	1.00	.00	1.00
'C5(G)	'	5.00	.00	.00	.00
'H1N1O2(G)	'	.00	1.00	2.00	1.00
'C1(G)	'	1.00	.00	.00	.00
'C1H1N1O1(G)	'	1.00	1.00	1.00	1.00
'H1(G)	'	.00	1.00	.00	.00
'H1N1(G)	'	.00	1.00	.00	1.00
'C1N2(G)	'	1.00	.00	.00	2.00
'C4(G)	'	4.00	.00	.00	.00
'C1H2O1(G)	'	1.00	2.00	1.00	.00
'N2O4(G)	'	.00	.00	4.00	2.00
'C2H2(G)	'	2.00	2.00	.00	.00
'C2H4O1(G)	'	2.00	4.00	1.00	.00
'C1N1O1(G)	'	1.00	.00	1.00	1.00
'C1N1(G)	'	1.00	.00	.00	1.00
'C1H3(G)	'	1.00	3.00	.00	.00
'N1O2(G)	'	.00	.00	2.00	1.00
'C1H1O1(G)	'	1.00	1.00	1.00	.00
'C1H1(G)	'	1.00	1.00	.00	.00
'H1O1(G)	'	.00	1.00	1.00	.00
'C1H2(G)	'	1.00	2.00	.00	.00
'O1(G)	'	.00	.00	1.00	.00
'H2N1(G)	'	.00	2.00	.00	1.00
'C1O2(G)	'	1.00	.00	2.00	.00
'N1O3(G)	'	.00	.00	3.00	1.00
'N2O3(G)	'	.00	.00	3.00	2.00
'N1O1(G)	'	.00	.00	1.00	1.00
'C1H4(G)	'	1.00	4.00	.00	.00
'N2O5(G)	'	.00	.00	5.00	2.00
'N3(G)	'	.00	.00	.00	3.00

'H2N2(G)	'	.00	2.00	.00	2.00
'N1(G)	'	.00	.00	.00	1.00
'H1O2(G)	'	.00	1.00	2.00	.00
'H2O2(G)	'	.00	2.00	2.00	.00
'H2O1(L,G)-C	'	.00	2.00	1.00	.00
'H4N2(G)	'	.00	4.00	.00	2.00
'H3N1(G)	'	.00	3.00	.00	1.00
'C1O1(G)	'	1.00	.00	1.00	.00
'O3(G)	'	.00	.00	3.00	.00
'C1(REF)'		1.	0.	0.	0.

```
54,2,3,1
6
1144.26
7
200.0
2
1
2 2 2 2
53.72
619.38
418.73
144.86
12
```

EXAMPLE 4: This example predicts the equilibrium
between a hydrated salt and its evolved
water vapor. Coefficients for C_p functions
are provided as thermochemical data. The
data deck causes SOLGASMIX to calculate
equilibria at 9 temperature/pressure points:
temperatures of 500, 600, and 700 K, with
pressures of 1.0, 1.5, and 2.0 atmospheres
for each temperature.

```
EXAMPLE 4: DEHYDRATION OF ALUMINUM OXIDE TRIHYDRATE.
3,2,0,3,5
'O','H','AL'
'OTWO'    2.0      0.0      0.0
'HTWO'    0.0      2.0      0.0
'H2O'     1.0      2.0      0.0
'AL'      0.0      0.0      1.0
'ANHYD'   3.0      0.0      2.0
'MONO'    4.0      2.0      2.0
'DIHYD'   5.0      4.0      2.0
'TRIHYD'  6.0      6.0      2.0
1,2,4
2
500.00
0.0                   205.13
0.0                   130.65
-242579.              188.81
0.0                   28.34
-1674400.             51.07
-1971606.             96.91
-2270500.             118.59
-2568948.             140.27
 1 1 1 1 1 1 1 1
29.972    4.186E-3   0.0   -1.67E5   0.0   0.0   0.0
27.293    3.265E-3   0.0    5.02E4   0.0   0.0   0.0
30.014    1.072E-3   0.0    3.35E4   0.0   0.0   0.0
20.679    1.237E-2   0.0    0.0      0.0   0.0   0.0
114.82    1.281E-2   0.0   -3.55E6   0.0   0.0   0.0
108.75    4.939E-2   0.0    3.35E5   0.0   0.0   0.0
85.00     2.344E-1   0.0    0.0      0.0   0.0   0.0
61.24     4.194E-4   0.0    0.0      0.0   0.0   0.0
1
1
1 1 1
70.0
60.0
20.0
10.0   0.0   0.10   0.0   0.10   1.0   2.0   6.0
6
600.
5
6
700.
```

5
7
1.500
6
500.
5
6
600.
5
6
700.
5
7
2.000
6
500.
5
6
600.
5
6
700.
5
10

EXAMPLE 5: In this example, the equilibrium between hydrogen, nitrogen, and ammonia is calculated. C_p functions are again used for thermochemical data input, and heat of reaction calculations are performed. Note that in an actual ammonia production process, a catalyst is needed due to a very slow rate of reaction.

```
EXAMPLE 5: AMMONIA EQUILIBRIUM, WITH HEAT.
2 1 0 3
            'N'        'H'
'NITROGEN' 2.0        0.0
'HYDROGEN' 0.0        2.0
'AMMONIA'  1.0        3.0
1,2
4
600.0
0.0      191.590
0.0      130.650
-46046.  192.430
1 1 1
27.67  0.4270E-2  0.0    0.0        0.0     0.0      0.0
27.29  0.3260E-2  0.0    0.5023E5   0.0     0.0      0.0
29.76  0.2512E-1  0.0   -0.1549E6   0.0     0.0      0.0
2 1 2
273.15
7
10.0
2
1
1  1
5.000
10.000
12
```

EXAMPLE 6: This is the same problem as in the previous
example, except the JANAF curvefit database is
used for thermochemical data. Note that the data
deck is significantly shorter, as there is no
need to enter coefficients for specific heat or
Gibbs free energy curves.

```
EXAMPLE 6: AMMONIA EQUILIBRIUM USING JANAF DATABASE
2 1 0 3
             'N'        'H'
'N2(REF)'    2.0        0.0
'H2(REF)'    0.0        2.0
'H3N1(G)'    1.0        3.0
1,2
5
600.0
2 1 2
273.15
7
10.0
2
1
2 2
5.000
10.000
12
```

EXAMPLE 7: This sample contains data for the equilibrium
between lithium and fluorine. Both C_p and
Gibbs free energy curvefits are specified, but
there is only one coefficient given for each
ΔG curve: thus, the data deck is valid at only
one temperature.

```
EXAMPLE 7: LITHIUM/FLUORINE REACTION.
2 2 0 4 2
           'LI'          'F'
'F2'       0.0          2.0
'LIF V'    1.0          1.0
'LI2F2'    2.0          2.0
'LI V'     1.0          0.0
'LI L'     1.0          0.0
'LIF L'    1.0          1.0
5 1
3
1 2
0.0
-410995.
-916769.
38285.
0.0
-503292.0
1200.
0.0            202.789
-340787.0      200.278
-942781.0      258.627
159300.0       138.781
2380.          33.938
-598651.0      42.962
1 1 1 1 1 1
34.440     0.0      0.0      0.0      0.0      0.0      0.0
34.302     0.0      0.0      0.0      0.0      0.0      0.0
72.291     0.0      0.0      0.0      0.0      0.0      0.0
20.786     0.0      0.0      0.0      0.0      0.0      0.0
30.018     0.0      0.0      0.0      0.0      0.0      0.0
64.183     0.0      0.0      0.0      0.0      0.0      0.0
2 1 5
298.15
2
1
1  1
1.0001
2.000
12
```

EXAMPLE 8: As in the previous example, this data deck solves
for the lithium/fluorine equilibrium. Note that
the JANAF curvefit database is utilized. Despite
having several additional species defined in the
system, this data deck is considerably shorter than
the previous one, illustrating the usefulness of
the database. Appendix B.2 is a listing of the
SOLGASMIX output produced by this example.

```
EXAMPLE 8: LITHIUM/FLUORINE SYSTEM, USING JANAF DATABASE
2,2,0,7,2
                                    'LI'    'F '
 'F2(REF)                    '  0.00    2.00
 'F1(G)                      '  0.00    1.00
 'F1LI1(G)                   '  1.00    1.00
 'F2LI2(G)                   '  2.00    2.00
 'F3LI3(G)                   '  3.00    3.00
 'LI1(G)                     '  1.00    0.00
 'LI2(G)                     '  2.00    0.00
 'LI1(L)                     '  1.00    0.00
 'F1LI1(L)                   '  1.00    1.00
8,1
5
1200.
2 1 8
298.15
1
1
2 2
1.0001
2.000
0.001   0.00   0.00   0.00   0.00   0.00 0.00 0.00 2.00
12
```

EXAMPLE 9: This example demonstrates several conditions under which incorrect results are obtained, and the methods used to correct for these results. See Appendix A.3 for a discussion. Note that the two user defined species "*(G)" and "**(CR)" are included in the dataset, necessitating the use of the JFIT program.

```
EXAMPLE 9: LI/H/O REACTION. KVAL2=-5
5,2,5,15,6
                   'H'      'O'      'LI'     '*'      '**'
'*(G)'             0.       0.       0.       1.0      0.
'H1(G)'            1.       0.       0.       0.       0.
'H2(REF)'          2.       0.       0.       0.       0.
'O1(G)'            0.       1.       0.       0.       0.
'O2(REF)'          0.       2.       0.       0.       0.
'H2O1(G)'          2.       1.       0.       0.       0.
'LI1(G)'           0.       0.       1.       0.       0.
'LI2(G)'           0.       0.       2.       0.       0.
'LI2O1(G)'         0.       1.       2.       0.       0.
'LI2O2(G)'         0.       2.       2.       0.       0.
'H1LI1(G)'         1.       0.       1.       0.       0.
'H1LI1O1(G)'       1.       1.       1.       0.       0.
'H2LI2O2(G)'       2.       2.       2.       0.       0.
'H1O1(G)'          1.       1.       0.       0.       0.
'H1O2(G)'          1.       2.       0.       0.       0.
'**(CR)'           0.       0.       0.       0.       1.
'LI1(L)'           0.       0.       1.       0.       0.
'H1LI1(L)'         1.       0.       1.       0.       0.
'H1LI1O1(L)'       1.       1.       1.       0.       0.
'LI2O1(L)'         0.       1.       2.       0.       0.
'H2O1(L)'          2.       1.       0.       0.       0.
'LI1(CR)'          0.       0.       1.       0.       0.
'H1LI1(CR)'        1.       0.       1.       0.       0.
'H1LI1O1(CR)'      1.       1.       1.       0.       0.
'LI2O1(CR)'        0.       1.       2.       0.       0.
'LI2O2(CR)'        0.       2.       2.       0.       0.
3,5,17,1,16
-5
1000.00
4   1   6   16   17
400.0
1
1
2 2 2 2
0.00
1.0
0.00
1.0
0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.0
1
```

```
1
2  2  2  2
0.00
1.0
0.001
1.0
0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.001  0.0    0.0    0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.0
1
1
2  2  2  2
0.0001
1.0
0.001
1.0
0.001  0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.001  0.0    0.0    0.0    0.0
0.0    0.0    0.0    0.0    0.0    0.0
10
```

APPENDIX B.2: EXAMPLE OF SOLGASMIX OUTPUT

EXAMPLE 8: LITHIUM/FLOURINE SYSTEM, USING JANAF DATABASE

NO. OF ELEMENTS = 2   NO. OF MIXTURES = 2   NO. OF INVARIANT SOLIDS = 0

NO. OF SPECIES PER MIXTURE = 7, 2.

SUBSCRIPTS ON ELEMENTAL SYMBOLS OF EACH SPECIES

	LI	F
F2(REF)	0.00	2.00
F1(G)	0.00	1.00
F1LI1(G)	1.00	1.00
F2LI2(G)	2.00	2.00
F3LI3(G)	3.00	3.00
LI1(G)	1.00	0.00
LI2(G)	2.00	0.00
LI1(L)	1.00	0.00
F1LI1(L)	1.00	1.00

EXAMPLE 8: LITHIUM/FLOURINE SYSTEM, USING JANAF DATABASE

STATISTICAL DATA FOR GIBB'S FREE ENERGY CURVEFITS

		# PTS	MAX TEMP	MAX % ERROR	MEAN % ERROR	STD DEV % ERROR	ABSOLUTE MAX ERROR (J/MOLE)
1	F2(REF)	23	2000.00	0.000	0.000	0.000	0.00000D+00
2	F1(G)	22	2000.00	0.126	0.006	0.027	0.19387D+01
3	F1LI1(G)	22	2000.00	0.789	0.016	0.285	0.33874D+04
4	F2LI2(G)	22	2000.00	0.752	0.017	0.276	0.67744D+04
5	F3LI3(G)	22	2000.00	0.751	0.018	0.277	0.10161D+05
6	LI1(G)	22	2000.00	0.213	0.009	0.071	0.15905D+03
7	LI2(G)	21	2000.00	19.190	0.121	5.609	0.67740D+04
8	LI1(L)	22	2000.00	35.800	1.841	7.660	0.23449D+03
9	F1LI1(L)	19	2000.00	0.711	0.026	0.285	0.32958D+04

EXAMPLE 8: LITHIUM/FLOURINE SYSTEM, USING JANAF DATABASE

COEFFICIENTS ON G(T) FUNCTIONS
$G(T)=A/T+B+CT+D(T^{*2})+E(T^{*3})+F(TLN\ )$

SPECIES	A	B	C	D	E	F
F2(REF)	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
F1(G)	-0.19270E+06	0.79390E+05	-0.29174E+02	0.14620E-02	-0.10987E-06	-0.46408E+01
F1LI1(G)	-0.27578E+08	0.36015E+05	-0.57897E+04	-0.80503E+00	0.12970E-03	0.87664E+03
F2LI2(G)	-0.54751E+08	-0.19501E+06	-0.11360E+05	-0.16080E+01	0.25924E-03	0.17423E+04
F3LI3(G)	-0.82114E+08	-0.39792E+06	-0.16919E+05	-0.24123E+01	0.38890E-03	0.26058E+04
LI1(G)	0.64263E+06	0.16288E+06	-0.28638E+03	-0.22493E-01	0.36378E-05	0.28753E+02
LI2(G)	-0.51947E+08	0.93508E+06	-0.11167E+05	-0.15719E+01	0.25522E-03	0.16930E+04
LI1(L)	0.47041E+08	-0.64021E+06	0.95054E+04	0.11834E+01	-0.14386E-03	-0.14434E+04
F1LI1(L)	-0.33209E+08	-0.17273E+06	-0.60897E+04	-0.86765E+00	0.13710E-03	0.94229E+03

VALUES FOR G(T) ARE IN J/MOLE

EXAMPLE 8: LITHIUM/FLOURINE SYSTEM, USING JANAF DATABASE

STATISTICAL DATA FOR H(T)-H(298) CURVEFITS

		MAX % ERROR	MEAN % ERROR	STD DEV % ERROR	ABSOLUTE MAX ERROR (J/MOLE)
1	F2(REF)	0.114	0.003	0.030	0.28700D+01
2	F1(G)	0.150	0.006	0.036	0.17686D+01
3	F1LI1(G)	0.153	0.009	0.035	0.25202D+01
4	F2LI2(G)	0.022	0.001	0.005	0.74824D+00
5	F3LI3(G)	0.022	0.001	0.005	0.11828D+01
6	LI1(G)	0.030	0.004	0.009	0.94230D+00
7	LI2(G)	0.945	0.039	0.245	0.18044D+02
8	LI1(L)	0.584	0.016	0.139	0.14227D+02
9	F1LI1(L)	0.057	0.004	0.013	0.37050D+01

EXAMPLE 8: LITHIUM/FLOURINE SYSTEM, USING JANAF DATABASE

	HF(298) J/(MOL)	# CURVES	TRANSITION TEMPERATURES (K)
F2(REF)	0.	1	
F1(G)	79390.	1	
F1LI1(C)	-340787.	1	
F2LI2(G)	-942781.	1	
F3LI3(G)	-1517202.	1	
LI1(G)	159300.	1	
LI2(G)	215900.	1	
LI1(L)	2380.	1	
F1LI1(L)	-598651.		

EXAMPLE 8: LITHIUM/FLOURINE SYSTEM, USING JANAF DATABASE

COEFFICIENTS ON H(T)-H(298) FUNCTIONS
H(T)-H(298)=A+BT+C(T**2)+D(T**3)+E/T+F/(T**2)

SPECIES	A	B	C	D	E	F
F2(REF)	-0.13421E+05	0.36142E+02	0.10411E-02	-0.97373E-07	0.10363E+07	-0.81815E+08
F1(G)	-0.51632E+04	0.21028E+02	-0.10709E-03	0.18014E-07	-0.50530E+06	0.53128E+08
F1LI1(G)	-0.14381E+05	0.37400E+02	0.31491E-03	-0.75828E-08	0.13641E+07	-0.12212E+09
F2LI2(G)	-0.32934E+05	0.83672E+02	-0.21119E-03	0.33268E-07	0.29566E+07	-0.16991E+09
F3LI3(G)	-0.52365E+05	0.13381E+03	-0.31101E-03	0.49116E-07	0.46910E+07	-0.28789E+09
LI1(G)	-0.63222E+04	0.20970E+02	-0.12322E-03	0.30438E-07	0.38832E+05	0.44844E+07
LI2(G)	-0.13348E+05	0.37528E+02	0.26772E-02	-0.11061E-05	0.99801E+06	0.12432E+09
LI1(L)	-0.40698E+04	0.24573E+02	0.21517E-02	-0.45163E-06	-0.15812E+07	0.16603E+09
F1LI1(L)	-0.19343E+05	0.64404E+02	-0.10794E-03	0.19375E-07	0.85856E+05	-0.12270E+08

VALUES FOR H(T)-H(298) ARE IN J/MOLE

TO = 298.15 K

EXAMPLE 8: LITHIUM/FLOURINE SYSTEM, USING JANAF DATABASE

```
T = 1200.00 K                    T =   1700.33 F
P = 1.000D+00 ATM                P = 1.470D+01 PSIA
VOLUME = 1.230D-02 LITERS        VOLUME = 4.342D-04 FT**3

          MOLAR AMOUNTS:
           INITIAL       EQUILIBRIUM      P/ATM         ACTIVITY
F2(REF)    0.10001D+01   0.75132D-04   0.60155D+00   0.60155D+00
F1(G)      0.00000D+00   0.49737D-04   0.39822D+00   0.39822D+00
F1LI1(G)   0.00000D+00   0.11916D-07   0.95404D-04   0.95404D-04
F2LI2(G)   0.00000D+00   0.15183D-07   0.12156D-03   0.12156D-03
F3LI3(G)   0.00000D+00   0.21037D-08   0.16843D-04   0.16843D-04
LI1(G)     0.00000D+00   0.41951D-27   0.33589D-23   0.33589D-23
LI2(G)     0.00000D+00   0.19422D-50   0.15550D-46   0.15550D-46

           INITIAL       EQUILIBRIUM   MOLE FRACTION  ACTIVITY
LI1(L)     0.20000D+01   0.31211D-21   0.15605D-21   0.15605D-21
F1LI1(L)   0.00000D+00   0.20000D+01   0.10000D+01   0.10000D+01
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EXAMPLE 8: LITHIUM/FLOURINE SYSTEM, USING JANAF DATABASE

CALCULATED THERMOCHEMICAL DATA. T = 1200.00

SPECIES	H(T) - H(298)	HEAT OF FORMATION	ENTROPY OF FORMATION	GIBBS FREE ENERGY
F2(REF)	0.320870+05	0.000000+00	0.000000+00	0.000000+00
F1(G)	0.195630+05	0.829100+05	0.635490+02	0.665100+04
F1L11(G)	0.319930+05	-0.353750+06	0.478290+02	-0.411150+06
F2L12(G)	0.695720+05	-0.963120+06	0.381750+02	-0.917670+06
F3L13(G)	0.111560+06	-0.154050+07	-0.116380+03	-0.140050+07
L11(G)	0.187460+05	0.149130+06	0.923620+02	0.302980+05
L12(G)	0.343770+05	0.192450+06	0.992120+02	0.733960+05
L11(L)	0.265330+05	0.000000+00	0.000000+00	0.000000+00
F1L11(L)	0.578830+05	-0.585720+06	-0.685130+02	-0.503510+06

PRE-HEAT =   0.85200+02 KJ   8.07718D+01 BTU
HEAT OF REACTION = -1.17100+03 KJ   -1.11130+03 BTU
TOTAL HEAT =   -1.08600+03 KJ   -1.03035D+03 BTU

APPENDIX C: INDEX TO SPECIES IN JANAF CURVEFIT DATABASE.

AL1(CR)	ALUMINUM (AL)
AL1(CR,L)	ALUMINUM (AL)
AL1(G)	ALUMINUM (AL)
AL1(L)	ALUMINUM (AL)
AL1(REF)	ALUMINUM (AL)
AL1+(G)	ALUMINUM, ION (AL+)
AL1-(G)	ALUMINUM, ION (AL-)
AL1BR1(G)	ALUMINUM BROMIDE (ALLR)
AL1BR3(CR)	ALUMINUM BROMIDE (ALLR3)
AL1BR3(CR,L)	ALUMINUM BROMIDE (ALLR3)
AL1BR3(G)	ALUMINUM BROMIDE (ALLR3)
AL1BR3(L)	ALUMINUM BROMIDE (ALLR3)
AL1B1O2(G)	ALUMINUM BORATE (ALLO2)
AL1CL1(G)	ALUMINUM CHLORIDE (ALCL)
AL1CL1+(G)	ALUMINUM CHLORIDE, ION (ALCL+)
AL1CL1F1(G)	ALUMINUM CHLORIDE FLUORIDE (ALCLF)
AL1CL1F1+(G)	ALUMINUM CHLORIDE FLUORIDE, ION (ALCLF+)
AL1CL1F2(G)	ALUMINUM CHLORIDE FLUORIDE (ALCLF2)
AL1CL1O1(CR)	ALUMINUM CHLORIDE OXIDE (OALCL)
AL1CL1O1(G)	ALUMINUM CHLORIDE OXIDE (OALCL)
AL1CL2(G)	ALUMINUM CHLORIDE (ALCL2)
AL1CL2+(G)	ALUMINUM CHLORIDE, ION (ALCL2+)
AL1CL2-(G)	ALUMINUM CHLORIDE, ION (ALCL2-)
AL1CL2F1(G)	ALUMINUM CHLORIDE FLUORIDE (ALCL2F)
AL1CL3(CR)	ALUMINUM CHLORIDE (ALCL3)
AL1CL3(CR,L)	ALUMINUM CHLORIDE (ALCL3)
AL1CL3(G)	ALUMINUM CHLORIDE (ALCL3)
AL1CL3(L)	ALUMINUM CHLORIDE (ALCL3)
AL1CL4K1(CR)	POTASSIUM TETRACHLOROALUMINATE (KALCL4)
AL1CL4NA1(CR)	SODIUM TETRACHLOROALUMINATE (NAALCL4)
AL1CL6K3(CR)	POTASSIUM HEXACHLOROALUMINATE (K3ALCL6)
AL1CL6NA3(CR)	SODIUM HEXACHLOROALUMINATE (NA3ALCL6)
AL1F1(G)	ALUMINUM FLUORIDE (ALF)
AL1F1+(G)	ALUMINUM FLUORIDE, ION (ALF+)
AL1F1O1(G)	ALUMINUM FLUORIDE OXIDE (OALF)
AL1F2(G)	ALUMINUM FLUORIDE (ALF2)
AL1F2+(G)	ALUMINUM FLUORIDE, ION (ALF2+)
AL1F2-(G)	ALUMINUM FLUORIDE, ION (ALF2-)
AL1F2O1(G)	ALUMINUM FLUORIDE OXIDE (OALF2)
AL1F2O1-(G)	ALUMINUM FLUORIDE OXIDE, ION (OALF2-)
AL1F3(CR)	ALUMINUM FLUORIDE (ALF3)
AL1F3(CR,L)	ALUMINUM FLUORIDE (ALF3)
AL1F3(G)	ALUMINUM FLUORIDE (ALF3)
AL1F3(L)	ALUMINUM FLUORIDE (ALF3)
AL1F4-(G)	TETRAFLUOROALUMINATE, ION (ALF4-)
AL1F4LI1(G)	LITHIUM TETRAFLUOROALUMINATE (LIALF4)
AL1F4NA1(G)	SODIUM TETRAFLUOROALUMINATE (NAALF4)
AL1F6K3(CR)	POTASSIUM HEXAFLUOROALUMINATE (K3ALF6)
AL1F6LI3(CR)	LITHIUM HEXAFLUOROALUMINATE (LI3ALF6)
AL1F6LI3(CR,L)	LITHIUM HEXAFLUOROALUMINATE (LI3ALF6)
AL1F6LI3(L)	LITHIUM HEXAFLUOROALUMINATE (LI3ALF6)

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AL1F6NA3(CR)            CRYOLITE, ALPHA (NA3ALF6)
AL1F6NA3(CR)-B          CRYOLITE, BETA (NA3ALF6)
AL1F6NA3(CR,L)          CRYOLITE (NA3ALF6)
AL1F6NA3(L)             CRYOLITE (NA3ALF6)
AL1H1(G)                ALUMINUM HYDRIDE (ALH)
AL1H1O1(G)              ALUMINUM HYDRIDE OXIDE (OALH)
AL1H1O1(G)-B            ALUMINUM HYDROXIDE (ALOH)
AL1H1O1+(G)             ALUMINUM HYDROXIDE, ION (ALOH+)
AL1H1O1-(G)             ALUMINUM HYDROXIDE, ION (ALOH-)
AL1H1O2(G)              ALUMINUM HYDROXIDE OXIDE (OALOH)
AL1H4LI1(CR)            LITHIUM TETRAHYDROALUMINATE (LIALH4)
AL1I1(G)                ALUMINUM IODIDE (ALI)
AL1I3(CR)               ALUMINUM IODIDE (ALI3)
AL1I3(CR,L)             ALUMINUM IODIDE (ALI3)
AL1I3(G)                ALUMINUM IODIDE (ALI3)
AL1I3(L)                ALUMINUM IODIDE (ALI3)
AL1LI1O2(CR)            LITHIUM ALUMINUM OXIDE (LIALO2)
AL1LI1O2(CR,L)          LITHIUM ALUMINUM OXIDE (LIALO2)
AL1LI1O2(L)             LITHIUM ALUMINUM OXIDE (LIALO2)
AL1NA1O2(CR)            SODIUM ALUMINUM OXIDE (NAALO2)
AL1N1(CR)               ALUMINUM NITRIDE (ALN)
AL1N1(G)                ALUMINUM NITRIDE (ALN)
AL1O1(G)                ALUMINUM OXIDE (ALO)
AL1O1+(G)               ALUMINUM OXIDE, ION (ALO+)
AL1O1-(G)               ALUMINUM OXIDE, ION (ALO-)
AL1O2(G)                ALUMINUM OXIDE (ALO2)
AL1O2-(G)               ALUMINUM OXIDE, ION (ALO2-)
AL1S1(G)                ALUMINUM SULFIDE (ALS)
AL2(G)                  ALUMINUM (AL2)
AL2BE1O4(CR)            BERYLLIUM ALUMINUM OXIDE (BEAL2O4)
AL2BE1O4(CR,L)          BERYLLIUM ALUMINUM OXIDE (BEAL2O4)
AL2BE1O4(L)             BERYLLIUM ALUMINUM OXIDE (BEAL2O4)
AL2BR6(G)               ALUMINUM BROMIDE ((ALLR3)2)
AL2CL6(G)               ALUMINUM CHLORIDE ((ALCL3)2)
AL2CL9K3(CR)            POTASSIUM ALUMINUM CHLORIDE (K3AL2CL9)
AL2F6(G)                ALUMINUM FLUORIDE ((ALF3)2)
AL2I6(G)                ALUMINUM IODIDE ((ALI3)2)
AL2MG1O4(CR)            MAGNESIUM ALUMINUM OXIDE (MGAL2O4)
AL2MG1O4(CR,L)          MAGNESIUM ALUMINUM OXIDE (MGAL2O4)
AL2MG1O4(L)             MAGNESIUM ALUMINUM OXIDE (MGAL2O4)
AL2O1(G)                ALUMINUM OXIDE (AL2O)
AL2O1+(G)               ALUMINUM OXIDE, ION (AL2O+)
AL2O2(G)                ALUMINUM OXIDE ((ALO)2)
AL2O2+(G)               ALUMINUM OXIDE, ION (AL2O2+)
AL2O3(CR)               ALUMINUM OXIDE, ALPHA (AL2O3)
AL2O3(CR)-B             ALUMINUM OXIDE, DELTA (AL2O3)
AL2O3(CR)-C             ALUMINUM OXIDE, GAMMA (AL2O3)
AL2O3(CR)-D             ALUMINUM OXIDE, KAPPA (AL2O3)
AL2O3(CR,L)             ALUMINUM OXIDE (AL2O3)
AL2O3(L)                ALUMINUM OXIDE (AL2O3)
AL2O5SI1(CR)            ALUMINUM SILICATE, ANDALUSITE (AL2SIO5)
AL2O5SI1(CR)-B          ALUMINUM SILICATE, KYANITE (AL2SIO5)
AL2O5SI1(CR)-C          ALUMINUM SILICATE, SILLIMANITE (AL2SIO5)
AL2S3(CR)               ALUMINUM SULFIDE (AL2S3)
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AL3F14NA5(CR)              CHIOLITE (NA5AL3F14)
AL3F14NA5(CR,L)            CHIOLITE (NA5AL3F14)
AL3F14NA5(L)               CHIOLITE (NA5AL3F14)
AL6BE1O10(CR)              BERYLLIUM ALUMINUM OXIDE (BEAL6O10)
AL6BE1O10(CR,L)            BERYLLIUM ALUMINUM OXIDE (BEAL6O10)
AL6BE1O10(L)               BERYLLIUM ALUMINUM OXIDE (BEAL6O10)
AL6O13SI2(CR)              ALUMINUM SILICATE, MULLITE (AL6SI2O13)
AR1(REF)                   ARGON (AR)
AR1+(G)                    ARGON, ION (AR+)
BA1(CR)                    BARIUM (BA)
BA1(CR,L)                  BARIUM (BA)
BA1(G)                     BARIUM (BA)
BA1(L)                     BARIUM (BA)
BA1(REF)                   BARIUM (BA)
BA1+(G)                    BARIUM, ION (BA+)
BA1BR1(G)                  BARIUM BROMIDE (BABR)
BA1BR2(CR)                 BARIUM BROMIDE (BABR2)
BA1BR2(CR,L)               BARIUM BROMIDE (BABR2)
BA1BR2(G)                  BARIUM BROMIDE (BABR2)
BA1BR2(L)                  BARIUM BROMIDE (BABR2)
BA1CL1(G)                  BARIUM CHLORIDE (BACL)
BA1CL2(CR)                 BARIUM CHLORIDE (BACL2)
BA1CL2(CR,L)               BARIUM CHLORIDE (BACL2)
BA1CL2(G)                  BARIUM CHLORIDE (BACL2)
BA1CL2(L)                  BARIUM CHLORIDE (BACL2)
BA1F1(G)                   BARIUM FLUORIDE (BAF)
BA1F1+(G)                  BARIUM FLUORIDE, ION (BAF+)
BA1F2(CR)                  BARIUM FLUORIDE (BAF2)
BA1F2(CR,L)                BARIUM FLUORIDE (BAF2)
BA1F2(G)                   BARIUM FLUORIDE (BAF2)
BA1F2(L)                   BARIUM FLUORIDE (BAF2)
BA1H1O1(G)                 BARIUM HYDROXIDE (BAOH)
BA1H1O1+(G)                BARIUM HYDROXIDE, ION (BAOH+)
BA1H2O2(CR)                BARIUM HYDROXIDE, ALPHA (BA(OH)2)
BA1H2O2(CR,L)              BARIUM HYDROXIDE (BA(OH)2)
BA1H2O2(G)                 BARIUM HYDROXIDE (BA(OH)2)
BA1H2O2(L)                 BARIUM HYDROXIDE (BA(OH)2)
BA1I1(G)                   BARIUM IODIDE (BAI)
BA1I2(CR)                  BARIUM IODIDE (BAI2)
BA1I2(CR,L)                BARIUM IODIDE (BAI2)
BA1I2(G)                   BARIUM IODIDE (BAI2)
BA1I2(L)                   BARIUM IODIDE (BAI2)
BA1O1(CR)                  BARIUM OXIDE (BAO)
BA1O1(CR,L)                BARIUM OXIDE (BAO)
BA1O1(G)                   BARIUM OXIDE (BAO)
BA1O1(L)                   BARIUM OXIDE (BAO)
BA1S1(CR)                  BARIUM SULFIDE (BAS)
BA1S1(G)                   BARIUM SULFIDE (BAS)
BE1(CR)                    BERYLLIUM (BE)
BE1(CR,L)                  BERYLLIUM (BE)
BE1(G)                     BERYLLIUM (BE)
BE1(L)                     BERYLLIUM (BE)
BE1(REF)                   BERYLLIUM (BE)
BE1+(G)                    BERYLLIUM, ION (BE+)
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BE1BR1(G)                      BERYLLIUM BROMIDE (BEBR)
BE1BR2(CR)                     BERYLLIUM BROMIDE (BEBR2)
BE1BR2(G)                      BERYLLIUM BROMIDE (BEBR2)
BE1CL1(G)                      BERYLLIUM CHLORIDE (BECL)
BE1CL1+(G)                     BERYLLIUM CHLORIDE, ION (BECL+)
BE1CL1F1(G)                    BERYLLIUM CHLORIDE FLUORIDE (BECLF)
BE1CL2(CR)                     BERYLLIUM CHLORIDE, ALPHA (BECL2)
BE1CL2(CR)-B                   BERYLLIUM CHLORIDE, BETA (BECL2)
BE1CL2(CR,L)                   BERYLLIUM CHLORIDE (BECL2)
BE1CL2(G)                      BERYLLIUM CHLORIDE (BECL2)
BE1CL2(L)                      BERYLLIUM CHLORIDE (BECL2)
BE1F1(G)                       BERYLLIUM FLUORIDE (BEF)
BE1F2(CR)                      BERYLLIUM FLUORIDE (BEF2)
BE1F2(CR,L)                    BERYLLIUM FLUORIDE (BEF2)
BE1F2(G)                       BERYLLIUM FLUORIDE (BEF2)
BE1F2(L)                       BERYLLIUM FLUORIDE (BEF2)
BE1F3LI1(CR)                   LITHIUM TRIFLUOROBERYLLATE (LIBEF3)
BE1F3LI1(CR,L)                 LITHIUM TRIFLUOROBERYLLATE (LIBEF3)
BE1F3LI1(G)                    LITHIUM TRIFLUOROBERYLLATE (LIBEF3)
BE1F3LI1(L)                    LITHIUM TRIFLUOROBERYLLATE (LIBEF3)
BE1F4LI2(CR)                   LITHIUM TETRAFLUOROBERYLLATE (LI2BEF4)
BE1F4LI2(CR,L)                 LITHIUM TETRAFLUOROBERYLLATE (LI2BEF4)
BE1F4LI2(L)                    LITHIUM TETRAFLUOROBERYLLATE (LI2BEF4)
BE1H1(G)                       BERYLLIUM HYDRIDE (BEH)
BE1H1+(G)                      BERYLLIUM HYDRIDE, ION (BEH+)
BE1H1O1(G)                     BERYLLIUM HYDROXIDE (BEOH)
BE1H1O1+(G)                    BERYLLIUM HYDROXIDE, ION (BEOH+)
BE1H2(G)                       BERYLLIUM HYDRIDE (BEH2)
BE1H2O2(CR)                    BERYLLIUM HYDROXIDE, ALPHA (BE(OH)2)
BE1H2O2(CR)-B                  BERYLLIUM HYDROXIDE, BETA (BE(OH)2)
BE1H2O2(G)                     BERYLLIUM HYDROXIDE (BE(OH)2)
BE1I1(G)                       BERYLLIUM IODIDE (BEI)
BE1I2(CR)                      BERYLLIUM IODIDE (BEI2)
BE1I2(CR,L)                    BERYLLIUM IODIDE (BEI2)
BE1I2(G)                       BERYLLIUM IODIDE (BEI2)
BE1I2(L)                       BERYLLIUM IODIDE (BEI2)
BE1N1(G)                       BERYLLIUM NITRIDE (BEN)
BE1O1(CR)                      BERYLLIUM OXIDE, ALPHA (BEO)
BE1O1(CR)-B                    BERYLLIUM OXIDE, BETA (BEO)
BE1O1(CR,L)                    BERYLLIUM OXIDE (BEO)
BE1O1(G)                       BERYLLIUM OXIDE (BEO)
BE1O1(L)                       BERYLLIUM OXIDE (BEO)
BE1O4S1(CR)                    BERYLLIUM SULFATE, ALPHA (BESO4)
BE1O4S1(CR)-B                  BERYLLIUM SULFATE, BETA (BESO4)
BE1O4S1(CR)-C                  BERYLLIUM SULFATE, GAMMA (BESO4)
BE1O4W1(CR)                    BERYLLIUM TUNGSTEN OXIDE (BEWO4)
BE1S1(CR)                      BERYLLIUM SULFIDE (BES)
BE1S1(G)                       BERYLLIUM SULFIDE (BES)
BE2(G)                         BERYLLIUM (BE2)
BE2CL4(G)                      BERYLLIUM CHLORIDE ((BECL2)2)
BE2F2O1(G)                     BERYLLIUM FLUORIDE OXIDE (O(BEF)2)
BE2O1(G)                       BERYLLIUM OXIDE (BE2O)
BE2O2(G)                       BERYLLIUM OXIDE ((BEO)2)
BE2O4SI1(CR)                   BERYLLIUM SILICATE (BE2SIO4)
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BE3N2(CR)              BERYLLIUM NITRIDE, ALPHA (BE3N2)
BE3N2(CR,L)            BERYLLIUM NITRIDE (BE3N2)
BE3N2(L)               BERYLLIUM NITRIDE (BE3N2)
BE3O3(G)               BERYLLIUM OXIDE ((BEO)3)
BE4O4(G)               BERYLLIUM OXIDE ((BEO)4)
BE5O5(G)               BERYLLIUM OXIDE ((BEO)5)
BE6O6(G)               BERYLLIUM OXIDE ((BEO)6)
BR1(G)                 BROMINE (BR)
BR1+(G)                BROMINE, ION (BR+)
BR1-(G)                BROMINE, ION (BR-)
BR1CA1(G)              CALCIUM BROMIDE (CABR)
BR1CL1(G)              BROMINE CHLORIDE (BRCL)
BR1F1(G)               BROMINE FLUORIDE (BRF)
BR1F3(G)               BROMINE FLUORIDE (BRF3)
BR1F5(G)               BROMINE FLUORIDE (BRF5)
BR1F5S1(G)             SULFUR BROMIDE FLUORIDE (SBRF5)
BR1HG1(G)              MERCURY BROMIDE (HGBR)
BR1H1(G)               HYDROGEN BROMIDE (HBR)
BR1H3SI1(G)            BROMOSILANE (SIH3BR)
BR1H4N1(CR)            AMMONIUM BROMIDE (NH4BR)
BR1I1(G)               IODINE BROMIDE (IBR)
BR1K1(CR)              POTASSIUM BROMIDE (KBR)
BR1K1(CR,L)            POTASSIUM BROMIDE (KBR)
BR1K1(G)               POTASSIUM BROMIDE (KBR)
BR1K1(L)               POTASSIUM BROMIDE (KBR)
BR1LI1(CR)             LITHIUM BROMIDE (LIBR)
BR1LI1(CR,L)           LITHIUM BROMIDE (LIBR)
BR1LI1(G)              LITHIUM BROMIDE (LIBR)
BR1LI1(L)              LITHIUM BROMIDE (LIBR)
BR1MG1(G)              MAGNESIUM BROMIDE (MGBR)
BR1MO1(G)              MOLYBDENUM BROMIDE (MOBR)
BR1NA1(CR)             SODIUM BROMIDE (NABR)
BR1NA1(CR,L)           SODIUM BROMIDE (NABR)
BR1NA1(G)              SODIUM BROMIDE (NABR)
BR1NA1(L)              SODIUM BROMIDE (NABR)
BR1N1(G)               BROMOIMIDOGEN (NBR)
BR1N1O1(G)             NITROSYL BROMIDE (ONBR)
BR1PB1(G)              LEAD BROMIDE (PLLR)
BR1P1(G)               PHOSPHORUS BROMIDE (PBR)
BR1SI1(G)              BROMOSILYLIDYNE (SIBR)
BR1SR1(G)              STRONTIUM BROMIDE (SRBR)
BR1TI1(G)              TITANIUM BROMIDE (TIBR)
BR1W1(G)               TUNGSTEN BROMIDE (WBR)
BR1ZR1(G)              ZIRCONIUM BROMIDE (ZRBR)
BR2(CR,L)              BROMINE (BR2)
BR2(G)                 BROMINE (BR2)
BR2(REF)               BROMINE (BR2)
BR2CA1(CR)             CALCIUM BROMIDE (CABR2)
BR2CA1(CR,L)           CALCIUM BROMIDE (CABR2)
BR2CA1(G)              CALCIUM BROMIDE (CABR2)
BR2CA1(L)              CALCIUM BROMIDE (CABR2)
BR2FE1(CR)             IRON BROMIDE (FEBR2)
BR2FE1(CR,L)           IRON BROMIDE (FEBR2)
BR2FE1(G)              IRON BROMIDE (FEBR2)
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BR2FE1(L)                IRON BROMIDE (FEBR2)
BR2HG1(CR)               MERCURY BROMIDE (HGBR2)
BR2HG1(CR,L)             MERCURY BROMIDE (HGBR2)
BR2HG1(G)                MERCURY BROMIDE (HGBR2)
BR2HG1(L)                MERCURY BROMIDE (HGBR2)
BR2HG2(CR)               MERCURY BROMIDE (HG2BR2)
BR2H2SI1(G)              DIBROMOSILANE (SIH2BR2)
BR2K2(G)                 POTASSIUM BROMIDE ((KBR)2)
BR2LI2(G)                LITHIUM BROMIDE ((LIBR)2)
BR2MG1(CR)               MAGNESIUM BROMIDE (MGBR2)
BR2MG1(CR,L)             MAGNESIUM BROMIDE (MGBR2)
BR2MG1(G)                MAGNESIUM BROMIDE (MGBR2)
BR2MG1(L)                MAGNESIUM BROMIDE (MGBR2)
BR2MG1+(G)               MAGNESIUM BROMIDE, ION (MGBR2+)
BR2MO1(CR)               MOLYBDENUM BROMIDE (MOBR2)
BR2MO1(G)                MOLYBDENUM BROMIDE (MOBR2)
BR2NA2(G)                SODIUM BROMIDE ((NABR)2)
BR2PB1(CR)               LEAD BROMIDE (PLLR2)
BR2PB1(CR,L)             LEAD BROMIDE (PLLR2)
BR2PB1(G)                LEAD BROMIDE (PLLR2)
BR2PB1(L)                LEAD BROMIDE (PLLR2)
BR2SI1(G)                DIBROMOSILYLENE (SIBR2)
BR2SR1(CR)               STRONTIUM BROMIDE (SRBR2)
BR2SR1(CR,L)             STRONTIUM BROMIDE (SRBR2)
BR2SR1(G)                STRONTIUM BROMIDE (SRBR2)
BR2SR1(L)                STRONTIUM BROMIDE (SRBR2)
BR2TI1(CR)               TITANIUM BROMIDE (TIBR2)
BR2TI1(G)                TITANIUM BROMIDE (TIBR2)
BR2ZR1(CR)               ZIRCONIUM BROMIDE (ZRBR2)
BR2ZR1(CR,L)             ZIRCONIUM BROMIDE (ZRBR2)
BR2ZR1(G)                ZIRCONIUM BROMIDE (ZRBR2)
BR2ZR1(L)                ZIRCONIUM BROMIDE (ZRBR2)
BR3H1SI1(G)              TRIBROMOSILANE (SIHBR3)
BR3MO1(CR)               MOLYBDENUM BROMIDE (MOBR3)
BR3MO1(G)                MOLYBDENUM BROMIDE (MOBR3)
BR3O1P1(G)               PHOSPHORYL BROMIDE (POBR3)
BR3P1(G)                 PHOSPHORUS BROMIDE (PBR3)
BR3P1S1(G)               THIOPHOSPHORYL BROMIDE (PSBR3)
BR3SI1(G)                TRIBROMOSILYL (SIBR3)
BR3TI1(CR)               TITANIUM BROMIDE (TIBR3)
BR3TI1(G)                TITANIUM BROMIDE (TIBR3)
BR3ZR1(CR)               ZIRCONIUM BROMIDE (ZRBR3)
BR3ZR1(G)                ZIRCONIUM BROMIDE (ZRBR3)
BR4FE2(G)                IRON BROMIDE ((FEBR2)2)
BR4MG2(G)                MAGNESIUM BROMIDE ((MGBR2)2)
BR4MO1(CR)               MOLYBDENUM BROMIDE (MOBR4)
BR4MO1(G)                MOLYBDENUM BROMIDE (MOBR4)
BR4PB1(G)                LEAD BROMIDE (PLLR4)
BR4SI1(G)                TETRABROMOSILANE (SIBR4)
BR4SI1(L)                TETRABROMOSILANE (SIBR4)
BR4TI1(CR)               TITANIUM BROMIDE (TIBR4)
BR4TI1(CR,L)             TITANIUM BROMIDE (TIBR4)
BR4TI1(G)                TITANIUM BROMIDE (TIBR4)
BR4TI1(L)                TITANIUM BROMIDE (TIBR4)
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BR4ZR1(CR)	ZIRCONIUM BROMIDE (ZRBR4)
BR4ZR1(G)	ZIRCONIUM BROMIDE (ZRBR4)
BR5NB1(CR)	NIOBIUM BROMIDE (NLLR5)
BR5NB1(CR,L)	NIOBIUM BROMIDE (NLLR5)
BR5NB1(G)	NIOBIUM BROMIDE (NLLR5)
BR5NB1(L)	NIOBIUM BROMIDE (NLLR5)
BR5W1(CR)	TUNGSTEN BROMIDE (WBR5)
BR5W1(CR,L)	TUNGSTEN BROMIDE (WBR5)
BR5W1(G)	TUNGSTEN BROMIDE (WBR5)
BR5W1(L)	TUNGSTEN BROMIDE (WBR5)
BR6W1(CR)	TUNGSTEN BROMIDE (WBR6)
BR6W1(G)	TUNGSTEN BROMIDE (WBR6)
B1(CR)	BORON, BETA-RHOMBOHEDRAL (B)
B1(CR,L)	BORON (B)
B1(G)	BORON (B)
B1(L)	BORON (B)
B1(REF)	BORON (B)
B1+(G)	BORON, ION (B+)
B1-(G)	BORON, ION (B-)
B1BE1O2(G)	BERYLLIUM BORATE (BEBO2)
B1BR1(G)	BROMOBORANE (LLR)
B1BR1CL1(G)	BROMOCHLOROBORANE (LLRCL)
B1BR1CL2(G)	BROMODICHLOROBORANE (LLRCL2)
B1BR1F1(G)	BROMOFLUOROBORANE (LLRF)
B1BR1F2(G)	BROMODIFLUOROBORANE (LLRF2)
B1BR1O1(G)	BORON BROMIDE OXIDE (OLLR)
B1BR2(G)	DIBROMOBORANE (LLR2)
B1BR2CL1(G)	DIBROMOCHLOROBORANE (LLR2CL)
B1BR2F1(G)	DIBROMOFLUOROBORANE (LLR2F)
B1BR2H1(G)	DIBROMOBORANE (BHBR2)
B1BR3(G)	TRIBROMOBORANE (LLR3)
B1BR3(L)	TRIBROMOBORANE (LLR3)
B1CL1(G)	CHLOROBORANE (BCL)
B1CL1+(G)	CHLOROBORANE, ION (BCL+)
B1CL1F1(G)	CHLOROFLUOROBORANE (BCLF)
B1CL1F2(G)	CHLORODIFLUOROBORANE (BCLF2)
B1CL1O1(G)	BORON CHLORIDE OXIDE (OBCL)
B1CL2(G)	DICHLOROBORANE (BCL2)
B1CL2+(G)	DICHLOROBORANE, ION (BCL2+)
B1CL2-(G)	DICHLOROBORANE, ION (BCL2-)
B1CL2F1(G)	DICHLOROFLUOROBORANE (BCL2F)
B1CL2H1(G)	DICHLOROBORANE (BHCL2)
B1CL3(G)	TRICHLOROBORANE (BCL3)
B1F1(G)	FLUOROBORANE (BF)
B1F1O1(G)	BORON FLUORIDE OXIDE (OBF)
B1F2(G)	DIFLUOROBORANE (BF2)
B1F2+(G)	DIFLUOROBORANE, ION (BF2+)
B1F2-(G)	DIFLUOROBORANE, ION (BF2-)
B1F2H1(G)	DIFLUOROBORANE (BHF2)
B1F2H1O1(G)	DIFLUOROHYDROXYBORANE (BF2OH)
B1F2O1(G)	BORON FLUORIDE OXIDE (OBF2)
B1F3(G)	TRIFLUOROBORANE (BF3)
B1F4K1(CR)	POTASSIUM TETRAFLUOROBORATE (KBF4)
B1F4K1(CR,L)	POTASSIUM TETRAFLUOROBORATE (KBF4)

B1F4K1(G)	POTASSIUM TETRAFLUOROBORATE (KBF4)
B1F4K1(L)	POTASSIUM TETRAFLUOROBORATE (KBF4)
B1H1(G)	BORANE (BH)
B1H1O1(G)	BORON HYDRIDE OXIDE (HBO)
B1H1O1+(G)	BORON HYDRIDE OXIDE, ION (HBO+)
B1H1O1-(G)	BORON HYDRIDE OXIDE, ION (HBO-)
B1H1O2(CR)	BORIC ACID (HBO2)
B1H1O2(G)	BORIC ACID (HBO2)
B1H1S1(G)	BORON HYDRIDE SULFIDE (HBS)
B1H1S1+(G)	BORON HYDRIDE SULFIDE, ION (HBS+)
B1H2(G)	BORANE (BH2)
B1H2O2(G)	DIHYDROXYBORANE (B(OH)2)
B1H3(G)	BORANE (BH3)
B1H3O3(CR)	BORIC ACID (H3BO3)
B1H3O3(G)	BORIC ACID (H3BO3)
B1H4K1(CR)	POTASSIUM TETRAHYDROBORATE (KBH4)
B1H4LI1(CR)	LITHIUM TETRAHYDROBORATE (LIBH4)
B1H4NA1(CR)	SODIUM TETRAHYDROBORATE (NABH4)
B1I1(G)	IODOBORANE (BI)
B1I2(G)	DIIODOBORANE (BI2)
B1I3(G)	TRIIODOBORANE (BI3)
B1K1O2(CR)	POTASSIUM BORATE (KBO2)
B1K1O2(CR,L)	POTASSIUM BORATE (KBO2)
B1K1O2(G)	POTASSIUM BORATE (KBO2)
B1K1O2(L)	POTASSIUM BORATE (KBO2)
B1LI1O2(CR)	LITHIUM BORATE (LIBO2)
B1LI1O2(CR,L)	LITHIUM BORATE (LIBO2)
B1LI1O2(G)	LITHIUM BORATE (LIBO2)
B1LI1O2(L)	LITHIUM BORATE (LIBO2)
B1NA1O2(CR)	SODIUM BORATE (NABO2)
B1NA1O2(CR,L)	SODIUM BORATE (NABO2)
B1NA1O2(G)	SODIUM BORATE (NABO2)
B1NA1O2(L)	SODIUM BORATE (NABO2)
B1N1(CR)	BORON NITRIDE (BN)
B1N1(G)	BORON NITRIDE (BN)
B1O1(G)	BORON OXIDE (BO)
B1O2(G)	BORON OXIDE (BO2)
B1O2-(G)	BORON OXIDE, ION (BO2-)
B1S1(G)	BORON SULFIDE (BS)
B1TI1(CR)	TITANIUM BORIDE (TIB)
B10H14(CR)	DECABORANE (B10H14)
B10H14(CR,L)	DECABORANE (B10H14)
B10H14(G)	DECABORANE (B10H14)
B10H14(L)	DECABORANE (B10H14)
B10O17PB2(CR)	LEAD BORATE (PB2B10O17)
B2(G)	BORON (B2)
B2BE1O4(G)	BERYLLIUM BORATE (BE(BO2)2)
B2BE3O6(CR)	BERYLLIUM BORATE (BE3B2O6)
B2CL4(G)	DICHLOROBORANE ((BCL2)2)
B2F4(G)	DIFLUOROBORANE ((BF2)2)
B2F4O1(G)	DIFLUOROBORANE OXIDE (O(BF2)2)
B2H4O4(CR)	DIHYDROXYBORANE ((B(OH)2)2)
B2H4O4(G)	DIHYDROXYBORANE ((B(OH)2)2)
B2H6(G)	DIBORANE (B2H6)

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B2MG1(CR)              MAGNESIUM BORIDE (MGB2)
B2O1(G)                BORON OXIDE (B2O)
B2O2(G)                BORON OXIDE ((BO)2)
B2O3(CR)               BORON OXIDE (B2O3)
B2O3(CR,L)             BORON OXIDE (B2O3)
B2O3(G)                BORON OXIDE (B2O3)
B2O3(L)                BORON OXIDE (B2O3)
B2O4PB1(CR)            LEAD BORATE (PLL2O4)
B2TI1(CR)              TITANIUM BORIDE (TIB2)
B2TI1(CR,L)            TITANIUM BORIDE (TIB2)
B2TI1(L)               TITANIUM BORIDE (TIB2)
B2ZR1(CR)              ZIRCONIUM BORIDE (ZRB2)
B2ZR1(CR,L)            ZIRCONIUM BORIDE (ZRB2)
B2ZR1(L)               ZIRCONIUM BORIDE (ZRB2)
B3CL3O3(G)             TRICHLOROBOROXIN (B3O3CL3)
B3F1H2O3(G)            FLUOROBOROXIN (B3H2O3F)
B3F2H1O3(G)            DIFLUOROBOROXIN (B3HO3F2)
B3F3O3(CR)             TRIFLUOROBOROXIN (B3O3F3)
B3F3O3(G)              TRIFLUOROBOROXIN (B3O3F3)
B3H3O3(CR)             BOROXIN (B3H3O3)
B3H3O3(G)              BOROXIN (B3H3O3)
B3H3O6(G)              BORIC ACID ((HBO2)3)
B3H6N3(G)              BORAZINE (B3H6N3)
B4K2O7(CR)             POTASSIUM BORATE (K2B4O7)
B4K2O7(CR,L)           POTASSIUM BORATE (K2B4O7)
B4K2O7(L)              POTASSIUM BORATE (K2B4O7)
B4LI2O7(CR)            LITHIUM BORATE (LI2B4O7)
B4LI2O7(CR,L)          LITHIUM BORATE (LI2B4O7)
B4LI2O7(L)             LITHIUM BORATE (LI2B4O7)
B4MG1(CR)              MAGNESIUM BORIDE (MGB4)
B4NA2O7(CR)            SODIUM BORATE (NA2B4O7)
B4NA2O7(CR,L)          SODIUM BORATE (NA2B4O7)
B4NA2O7(L)             SODIUM BORATE (NA2B4O7)
B4O7PB1(CR)            LEAD BORATE (PLL4O7)
B5H9(G)                PENTABORANE (B5H9)
B5H9(L)                PENTABORANE (B5H9)
B6K2O10(CR)            POTASSIUM BORATE (K2B6O10)
B6LI2O10(CR)           LITHIUM BORATE (LI2B6O10)
B6NA2O10(CR)           SODIUM BORATE (NA2B6O10)
B6O10PB1(CR)           LEAD BORATE (PLL6O10)
B8K2O13(CR)            POTASSIUM BORATE (K2B8O13)
B8K2O13(CR,L)          POTASSIUM BORATE (K2B8O13)
B8K2O13(L)             POTASSIUM BORATE (K2B8O13)
B8LI2O13(CR)           LITHIUM BORATE (LI2B8O13)
CA1(CR)                CALCIUM, ALPHA (CA)
CA1(CR)-B              CALCIUM, BETA (CA)
CA1(CR,L)              CALCIUM (CA)
CA1(G)                 CALCIUM (CA)
CA1(L)                 CALCIUM (CA)
CA1(REF)               CALCIUM (CA)
CA1+(G)                CALCIUM, ION (CA+)
CA1CL1(G)              CALCIUM CHLORIDE (CACL)
CA1CL2(CR)             CALCIUM CHLORIDE (CACL2)
CA1CL2(CR,L)           CALCIUM CHLORIDE (CACL2)
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CA1CL2(G)           CALCIUM CHLORIDE (CACL2)
CA1CL2(L)           CALCIUM CHLORIDE (CACL2)
CA1F1(G)            CALCIUM FLUORIDE (CAF)
CA1F2(CR)           CALCIUM FLUORIDE (CAF2)
CA1F2(CR,L)         CALCIUM FLUORIDE (CAF2)
CA1F2(G)            CALCIUM FLUORIDE (CAF2)
CA1F2(L)            CALCIUM FLUORIDE (CAF2)
CA1H1O1(G)          CALCIUM HYDROXIDE (CAOH)
CA1H1O1+(G)         CALCIUM HYDROXIDE, ION (CAOH+)
CA1H2O2(CR)         CALCIUM HYDROXIDE (CA(OH)2)
CA1H2O2(G)          CALCIUM HYDROXIDE (CA(OH)2)
CA1I1(G)            CALCIUM IODIDE (CAI)
CA1I2(CR)           CALCIUM IODIDE (CAI2)
CA1I2(CR,L)         CALCIUM IODIDE (CAI2)
CA1I2(G)            CALCIUM IODIDE (CAI2)
CA1I2(L)            CALCIUM IODIDE (CAI2)
CA1O1(CR)           CALCIUM OXIDE (CAO)
CA1O1(CR,L)         CALCIUM OXIDE (CAO)
CA1O1(G)            CALCIUM OXIDE (CAO)
CA1O1(L)            CALCIUM OXIDE (CAO)
CA1S1(CR)           CALCIUM SULFIDE (CAS)
CA1S1(G)            CALCIUM SULFIDE (CAS)
CA2(G)              CALCIUM (CA2)
CL1(G)              CHLORINE (CL)
CL1+(G)             CHLORINE, ION (CL+)
CL1-(G)             CHLORINE, ION (CL-)
CL1CO1(G)           COBALT CHLORIDE (COCL)
CL1CS1(CR)          CESIUM CHLORIDE (CSCL)
CL1CS1(CR,L)        CESIUM CHLORIDE (CSCL)
CL1CS1(G)           CESIUM CHLORIDE (CSCL)
CL1CS1(L)           CESIUM CHLORIDE (CSCL)
CL1CU1(CR)          COPPER CHLORIDE (CUCL)
CL1CU1(CR,L)        COPPER CHLORIDE (CUCL)
CL1CU1(G)           COPPER CHLORIDE (CUCL)
CL1CU1(L)           COPPER CHLORIDE (CUCL)
CL1D1(G)            HYDROCHLORIC ACID-D (DCL)
CL1D1O1(G)          HYPOCHLOROUS ACID-D (DOCL)
CL1FE1(G)           IRON CHLORIDE (FECL)
CL1F1(G)            CHLORINE FLUORIDE (CLF)
CL1F1LI2(G)         LITHIUM CHLORIDE FLUORIDE (LI2CLF)
CL1F1MG1(G)         MAGNESIUM CHLORIDE FLUORIDE (MGCLF)
CL1F1O2S1(G)        SULFURYL CHLORIDE FLUORIDE (SO2CLF)
CL1F1O3(G)          PERCHLORYL FLUORIDE (CLO3F)
CL1F2O1P1(G)        PHOSPHORYL CHLORIDE FLUORIDE (POCLF2)
CL1F3(G)            CHLORINE FLUORIDE (CLF3)
CL1F3SI1(G)         CHLOROTRIFLUOROSILANE (SICLF3)
CL1F5(G)            CHLORINE FLUORIDE (CLF5)
CL1F5S1(G)          SULFUR CHLORIDE FLUORIDE (SCLF5)
CL1HG1(G)           MERCURY CHLORIDE (HGCL)
CL1H1(G)            HYDROGEN CHLORIDE (HCL)
CL1H1O1(G)          HYPOCHLOROUS ACID (HOCL)
CL1H3SI1(G)         CHLOROSILANE (SIH3CL)
CL1H4N1(CR)         AMMONIUM CHLORIDE (NH4CL)
CL1H4N1O4(CR)       AMMONIUM PERCHLORATE (NH4CLO4)
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CL1I1(CR)              IODINE CHLORIDE (ICL)
CL1I1(CR,L)            IODINE CHLORIDE (ICL)
CL1I1(G)               IODINE CHLORIDE (ICL)
CL1I1(L)               IODINE CHLORIDE (ICL)
CL1K1(CR)              POTASSIUM CHLORIDE (KCL)
CL1K1(CR,L)            POTASSIUM CHLORIDE (KCL)
CL1K1(G)               POTASSIUM CHLORIDE (KCL)
CL1K1(L)               POTASSIUM CHLORIDE (KCL)
CL1K1O4(CR)            POTASSIUM PERCHLORATE (KCLO4)
CL1LI1(CR)             LITHIUM CHLORIDE (LICL)
CL1LI1(CR,L)           LITHIUM CHLORIDE ((LICL)
CL1LI1(G)              LITHIUM CHLORIDE (LICL)
CL1LI1(L)              LITHIUM CHLORIDE (LICL)
CL1LI1O1(G)            LITHIUM HYPOCHLORITE (LIOCL)
CL1LI1O4(CR)           LITHIUM PERCHLORATE (LICLO4)
CL1LI1O4(CR,L)         LITHIUM PERCHLORATE (LICLO4)
CL1LI1O4(L)            LITHIUM PERCHLORATE (LICLO4)
CL1MG1(G)              MAGNESIUM CHLORIDE (MGCL)
CL1MG1+(G)             MAGNESIUM CHLORIDE, ION (MGCL+)
CL1NA1(CR)             SODIUM CHLORIDE (NACL)
CL1NA1(CR,L)           SODIUM CHLORIDE (NACL)
CL1NA1(G)              SODIUM CHLORIDE (NACL)
CL1NA1(L)              SODIUM CHLORIDE (NACL)
CL1NA1O4(CR)           SODIUM PERCHLORATE (NACLO4)
CL1NI1(G)              NICKEL CHLORIDE (NICL)
CL1N1O1(G)             NITROSYL CHLORIDE (ONCL)
CL1N1O2(G)             NITRYL CHLORIDE (NO2CL)
CL1O1(G)               CHLORINE OXIDE (CLO)
CL1O1TI1(G)            TITANIUM CHLORIDE OXIDE (OTICL)
CL1O2(G)               CHLORINE OXIDE (CLO2)
CL1PB1(G)              LEAD CHLORIDE (PBCL)
CL1PB1+(G)             LEAD CHLORIDE, ION (PBCL+)
CL1P1(G)               PHOSPHORUS CHLORIDE (PCL)
CL1SI1(G)              CLOROSILYLIDYNE (SICL)
CL1SR1(G)              STRONTIUM CHLORIDE (SRCL)
CL1S1(G)               SULFUR CHLORIDE (SCL)
CL1S1+(G)              SULFUR CHLORIDE, ION (SCL+)
CL1S2(G)               SULFUR CHLORIDE (S2CL)
CL1TI1(G)              TITANIUM CHLORIDE (TICL)
CL1W1(G)               TUNGSTEN CHLORIDE (WCL)
CL1ZR1(G)              ZIRCONIUM CHLORIDE (ZRCL)
CL10W2(G)              TUNGSTEN CHLORIDE ((WCL5)2)
CL2(REF)               CHLORINE (CL2)
CL2CO1(CR)             COBALT CHLORIDE (COCL2)
CL2CO1(CR,L)           COBALT CHLORIDE (COCL2)
CL2CO1(G)              COBALT CHLORIDE (COCL2)
CL2CO1(L)              COBALT CHLORIDE (COCL2)
CL2CS2(G)              CESIUM CHLORIDE ((CSCL)2)
CL2CU1(CR)             COPPER CHLORIDE (CUCL2)
CL2FE1(CR)             IRON CHLORIDE (FECL2)
CL2FE1(CR,L)           IRON CHLORIDE (FECL2)
CL2FE1(G)              IRON CHLORIDE (FECL2)
CL2FE1(L)              IRON CHLORIDE (FECL2)
CL2F1O1P1(G)           PHOSPHORYL CHLORIDE FLUORIDE (POCL2F)
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CL2HG1(CR)          MERCURY CHLORIDE (HGCL2)
CL2HG1(CR,L)        MERCURY CHLORIDE (HGCL2)
CL2HG1(G)           MERCURY CHLORIDE (HGCL2)
CL2HG1(L)           MERCURY CHLORIDE (HGCL2)
CL2HG2(CR)          MERCURY CHLORIDE (HG2CL2)
CL2H2SI1(G)         DICHLOROSILANE (SIH2CL2)
CL2K2(G)            POTASSIUM CHLORIDE ((KCL)2)
CL2LI2(G)           LITHIUM CHLORIDE ((LICL)2)
CL2MG1(CR)          MAGNESIUM CHLORIDE (MGCL2)
CL2MG1(CR,L)        MAGNESIUM CHLORIDE (MGCL2)
CL2MG1(G)           MAGNESIUM CHLORIDE (MGCL2)
CL2MG1(L)           MAGNESIUM CHLORIDE (MGCL2)
CL2MO1O2(G)         MOLYBDENUM CHLORIDE OXIDE (MOO2CL2)
CL2NA2(G)           SODIUM CHLORIDE ((NACL)2)
CL2NI1(CR)          NICKEL CHLORIDE (NICL2)
CL2NI1(CR,L)        NICKEL CHLORIDE (NICL2)
CL2NI1(G)           NICKEL CHLORIDE (NICL2)
CL2NI1(L)           NICKEL CHLORIDE (NICL2)
CL2O1(G)            CHLORINE OXIDE (CL2O)
CL2O1TI1(G)         TITANIUM CHLORIDE OXIDE (TIOCL2)
CL2O2S1(G)          SULFURYL CHLORIDE (SO2CL2)
CL2O2W1(CR)         TUNGSTEN CHLORIDE OXIDE (WO2CL2)
CL2O2W1(G)          TUNGSTEN CHLORIDE OXIDE (WO2CL2)
CL2PB1(CR)          LEAD CHLORIDE (PBCL2)
CL2PB1(CR,L)        LEAD CHLORIDE (PBCL2)
CL2PB1(G)           LEAD CHLORIDE (PBCL2)
CL2PB1(L)           LEAD CHLORIDE (PBCL2)
CL2PB1+(G)          LEAD CHLORIDE, ION (PBCL2+)
CL2SI1(G)           DICHLOROSILYLENE (SICL2)
CL2SR1(CR)          STRONTIUM CHLORIDE (SRCL2)
CL2SR1(CR,L)        STRONTIUM CHLORIDE (SRCL2)
CL2SR1(G)           STRONTIUM CHLORIDE (SRCL2)
CL2SR1(L)           STRONTIUM CHLORIDE (SRCL2)
CL2S1(G)            SULFUR CHLORIDE (SCL2)
CL2S1(L)            SULFUR CHLORIDE (SCL2)
CL2S1+(G)           SULFUR CHLORIDE, ION (SCL2+)
CL2S2(G)            SULFUR CHLORIDE (CLSSCL)
CL2S2(L)            SULFUR CHLORIDE (CLSSCL)
CL2TI1(CR)          TITANIUM CHLORIDE (TICL2)
CL2TI1(G)           TITANIUM CHLORIDE (TICL2)
CL2W1(CR)           TUNGSTEN CHLORIDE (WCL2)
CL2W1(G)            TUNGSTEN CHLORIDE (WCL2)
CL2ZR1(CR)          ZIRCONIUM CHLORIDE (ZRCL2)
CL2ZR1(CR,L)        ZIRCONIUM CHLORIDE (ZRCL2)
CL2ZR1(G)           ZIRCONIUM CHLORIDE (ZRCL2)
CL2ZR1(L)           ZIRCONIUM CHLORIDE (ZRCL2)
CL3CO1(G)           COBALT CHLORIDE (COCL3)
CL3CU3(G)           COPPER CHLORIDE ((CUCL)3)
CL3FE1(CR)          IRON CHLORIDE (FECL3)
CL3FE1(CR,L)        IRON CHLORIDE (FECL3)
CL3FE1(G)           IRON CHLORIDE (FECL3)
CL3FE1(L)           IRON CHLORIDE (FECL3)
CL3F1SI1(G)         TRICHLOROFLUOROSILANE (SICL3F)
CL3H1SI1(G)         TRICHLOROSILANE (SIHCL3)
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CL3LI3(G)	LITHIUM CHLORIDE ((LICL)3)
CL3O1P1(G)	PHOSPHORYL CHLORIDE (OPCL3)
CL3P1(G)	PHOSPHORUS CHLORIDE (PCL3)
CL3P1S1(G)	THIOPHOSPHORYL CHLORIDE (SPCL3)
CL3SI1(G)	TRICHLOROSILYL (SICL3)
CL3TI1(CR)	TITANIUM CHLORIDE (TICL3)
CL3TI1(G)	TITANIUM CHLORIDE (TICL3)
CL3ZR1(CR)	ZIRCONIUM CHLORIDE (ZRCL3)
CL3ZR1(G)	ZIRCONIUM CHLORIDE (ZRCL3)
CL4CO2(G)	COBALT CHLORIDE ((COCL2)2)
CL4FE2(G)	IRON CHLORIDE ((FECL2)2)
CL4MG2(G)	MAGNESIUM CHLORIDE ((MGCL2)2)
CL4MO1(CR)	MOLYBDENUM CHLORIDE (MOCL4)
CL4MO1(CR,L)	MOLYBDENUM CHLORIDE (MOCL4)
CL4MO1(G)	MOLYBDENUM CHLORIDE (MOCL4)
CL4MO1(L)	MOLYBDENUM CHLORIDE (MOCL4)
CL4O1W1(CR)	TUNGSTEN CHLORIDE OXIDE (OWCL4)
CL4O1W1(CR,L)	TUNGSTEN CHLORIDE OXIDE (OWCL4)
CL4O1W1(G)	TUNGSTEN CHLORIDE OXIDE (OWCL4)
CL4O1W1(L)	TUNGSTEN CHLORIDE OXIDE (OWCL4)
CL4PB1(G)	LEAD CHLORIDE (PBCL4)
CL4SI1(G)	TETRACHLOROSILANE (SICL4)
CL4TI1(CR)	TITANIUM CHLORIDE (TICL4)
CL4TI1(CR,L)	TITANIUM CHLORIDE (TICL4)
CL4TI1(G)	TITANIUM CHLORIDE (TICL4)
CL4TI1(L)	TITANIUM CHLORIDE (TICL4)
CL4W1(CR)	TUNGSTEN CHLORIDE (WCL4)
CL4W1(G)	TUNGSTEN CHLORIDE (WCL4)
CL4ZR1(CR)	ZIRCONIUM CHLORIDE (ZRCL4)
CL4ZR1(G)	ZIRCONIUM CHLORIDE (ZRCL4)
CL5MO1(CR)	MOLYBDENUM CHLORIDE (MOCL5)
CL5MO1(CR,L)	MOLYBDENUM CHLORIDE (MOCL5)
CL5MO1(G)	MOLYBDENUM CHLORIDE (MOCL5)
CL5MO1(L)	MOLYBDENUM CHLORIDE (MOCL5)
CL5NB1(CR)	NIOBIUM CHLORIDE (NBCL5)
CL5N31(CR,L)	NIOBIUM CHLORIDE (NBCL5)
CL5NB1(G)	NIOBIUM CHLORIDE (NBCL5)
CL5NB1(L)	NIOBIUM CHLORIDE (NBCL5)
CL5P1(G)	PHOSPHORUS CHLORIDE (PCL5)
CL5TA1(CR)	TANTALUM CHLORIDE (TACL5)
CL5TA1(CR,L)	TANTALUM CHLORIDE (TACL5)
CL5TA1(G)	TANTALUM CHLORIDE (TACL5)
CL5TA1(L)	TANTALUM CHLORIDE (TACL5)
CL5W1(CR)	TUNGSTEN CHLORIDE (WCL5)
CL5W1(CR,L)	TUNGSTEN CHLORIDE (WCL5)
CL5W1(G)	TUNGSTEN CHLORIDE (WCL5)
CL5W1(L)	TUNGSTEN CHLORIDE (WCL5)
CL6FE2(G)	IRON CHLORIDE ((FECL3)2)
CL6MO1(CR)	MOLYBDENUM CHLORIDE (MOCL6)
CL6MO1(G)	MOLYBDENUM CHLORIDE (MOCL6)
CL6W1(CR)	TUNGSTEN CHLORIDE, ALPHA (WCL6)
CL6W1(CR)-B	TUNGSTEN CHLORIDE, BETA (WCL6)
CL6W1(CR,L)	TUNGSTEN CHLORIDE (WCL6)
CL6W1(G)	TUNGSTEN CHLORIDE (WCL6)

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CL6W1(L)            TUNGSTEN CHLORIDE (WCL6)
CO1(CR)             COBALT (CO)
CO1(CR,L)           COBALT (CO)
CO1(G)              COBALT (CO)
CO1(L)              COBALT (CO)
CO1(REF)            COBALT (CO)
CO1+(G)             COBALT, ION (CO+)
CO1-(G)             COBALT, ION (CO-)
CO1F2(CR)           COBALT FLUORIDE (COF2)
CO1F2(CR,L)         COBALT FLUORIDE (COF2)
CO1F2(G)            COBALT FLUORIDE (COF2)
CO1F2(L)            COBALT FLUORIDE (COF2)
CO1F3(CR)           COBALT FLUORIDE (COF3)
CO1O1(CR)           COBALT OXIDE (COO)
CO1O4S1(CR)         COBALT SULFATE (COSO4)
CO3O4(CR)           COBALT OXIDE (CO3O4)
CR1(CR)             CHROMIUM (CR)
CR1(CR,L)           CHROMIUM (CR)
CR1(G)              CHROMIUM (CR)
CR1(L)              CHROMIUM (CR)
CR1(REF)            CHROMIUM (CR)
CR1+(G)             CHROMIUM, ION (CR+)
CR1-(G)             CHROMIUM, ION (CR-)
CR1N1(CR)           CHROMIUM NITRIDE (CRN)
CR1N1(G)            CHROMIUM NITRIDE (CRN)
CR1O1(G)            CHROMIUM OXIDE (CRO)
CR1O2(G)            CHROMIUM OXIDE (CRO2)
CR1O3(G)            CHROMIUM OXIDE (CRO3)
CR2N1(CR)           CHROMIUM NITRIDE (CR2N)
CR2O3(CR)           CHROMIUM OXIDE (CR2O3)
CR2O3(CR,L)         CHROMIUM OXIDE (CR2O3)
CR2O3(L)            CHROMIUM OXIDE (CR2O3)
CS1(CR)             CESIUM (CS)
CS1(CR,L)           CESIUM (CS)
CS1(G)              CESIUM (CS)
CS1(L)              CESIUM (CS)
CS1(REF)            CESIUM (CS)
CS1+(G)             CESIUM, ION (CS+)
CS1-(G)             CESIUM, ION  (CS-)
CS1F1(CR)           CESIUM FLUORIDE (CSF)
CS1F1(CR,L)         CESIUM FLUORIDE (CSF)
CS1F1(G)            CESIUM FLUORIDE (CSF)
CS1F1(L)            CESIUM FLUORIDE (CSF)
CS1H1O1(CR)         CESIUM HYDROXIDE (CSOH)
CS1H1O1(CR,L)       CESIUM HYDROXIDE (CSOH)
CS1H1O1(G)          CESIUM HYDROXIDE (CSOH)
CS1H1O1(L)          CESIUM HYDROXIDE (CSOH)
CS1H1O1+(G)         CESIUM HYDROXIDE, ION (CSOH+)
CS1O1(G)            CESIUM OXIDE (CSO)
CS2(G)              CESIUM (CS2)
CS2F2(G)            CESIUM FLUORIDE ((CSF)2)
CS2H2O2(G)          CESIUM HYDROXIDE ((CSOH)2)
CS2O1(G)            CESIUM OXIDE (CS2O)
CS2O4S1(CR)         CESIUM SULFATE, I (CS2SO4)
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CS2O4S1(CR)-B          CESIUM SULFATE, II (CS2SO4)
CS2O4S1(CR,L)          CESIUM SULFATE (CS2SO4)
CS2O4S1(G)             CESIUM SULFATE (CS2SO4)
CS2O4S1(L)             CESIUM SULFATE (CS2SO4)
CU1(CR)                COPPER (CU)
CU1(CR,L)              COPPER (CU)
CU1(G)                 COPPER (CU)
CU1(L)                 COPPER (CU)
CU1(REF)               COPPER (CU)
CU1+(G)                COPPER, ION (CU+)
CU1-(G)                COPPER, ION (CU-)
CU1F1(CR)              COPPER FLUORIDE (CUF)
CU1F1(G)               COPPER FLUORIDE (CUF)
CU1F2(CR)              COPPER FLUORIDE (CUF2)
CU1F2(CR,L)            COPPER FLUORIDE (CUF2)
CU1F2(G)               COPPER FLUORIDE (CUF2)
CU1F2(L)               COPPER FLUORIDE (CUF2)
CU1H2O2(CR)            COPPER HYDROXIDE (CU(OH)2)
CU1O1(CR)              COPPER OXIDE (CUO)
CU1O1(G)               COPPER OXIDE (CUO)
CU1O4S1(CR)            COPPER SULFATE (CUSO4)
CU2(G)                 COPPER (CU2)
CU2O1(CR)              COPPER OXIDE (CU2O)
CU2O1(CR,L)            COPPER OXIDE (CU2O)
CU2O1(L)               COPPER OXIDE (CU2O)
CU2O5S1(CR)            COPPER OXIDE SULFATE (CUO.CUSO4)
C0.98NB1(CR)           NIOBIUM CARBIDE (NBC0.98)
C1(G)                  CARBON (C)
C1(REF)                CARBON (C)
C1+(G)                 CARBON, ION (C+)
C1-(G)                 CARBON, ION (C-)
C1AL1(G)               ALUMINUM CARBIDE (ALC)
C1BE2(CR)              BERYLLIUM CARBIDE (BE2C)
C1BE2(CR,L)            BERYLLIUM CARBIDE (BE2C)
C1BE2(L)               BERYLLIUM CARBIDE (BE2C)
C1BR1(G)               BROMOMETHYLIDYNE (CBR)
C1BR1F3(G)             BROMOTRIFLUOROMETHANE (CBRF3)
C1BR1N1(G)             CYANOGEN BROMIDE (BRCN)
C1BR4(G)               TETRABROMOMETHANE (CBR4)
C1B1(G)                BORON CARBIDE (BC)
C1B4(CR)               BORON CARBIDE (B4C)
C1B4(CR,L)             BORON CARBIDE (B4C)
C1B4(L)                BORON CARBIDE (B4C)
C1CL1(G)               CHLOROMETHYLIDYNE (CCL)
C1CL1F1O1(G)           CARBONIC CHLORIDE FLUORIDE (COCLF)
C1CL1F3(G)             CHLOROTRIFLUOROMETHANE (CCLF3)
C1CL1N1(G)             CYANOGEN CHLORIDE (CLCN)
C1CL1O1(G)             CARBONYL CHLORIDE (COCL)
C1CL2(G)               DICHLOROMETHYLENE (CCL2)
C1CL2F2(G)             DICHLORODIFLUOROMETHANE (CCL2F2)
C1CL2O1(G)             CARBONIC DICHLORIDE (COCL2)
C1CL3(G)               TRICHLOROMETHYL (CCL3)
C1CL3F1(G)             TRICLOROFLUORMETHANE (CCL3F)
C1CL4(G)               TETRACHLOROMETHANE (CCL4)
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C1CU1N1(CR)                  COPPER CYANIDE (CUCN)
C1F1(G)                      FLUOROMETHYLIDYNE (CF)
C1F1+(G)                     FLUOROMETHYLIDYNE, ION (CF+)
C1F1N1(G)                    CYANOGEN FLUORIDE (FCN)
C1F1O1(G)                    CARBONYL FLUORIDE (COF)
C1F2(G)                      DIFLUOROMETHYLENE (CF2)
C1F2+(G)                     DIFLUOROMETHYLENE, ION (CF2+)
C1F2O1(G)                    CARBONIC DIFLUORIDE (COF2)
C1F3(G)                      TRIFLUOROMETHYL (CF3)
C1F3+(G)                     TRIFLUOROMETHYL, ION (CF3+)
C1F3I1(G)                    TRIFLUORIODOMETHANE (CIF3)
C1F4(G)                      TETRAFLUOROMETHANE (CF4)
C1F4O1(G)                    TRIFLUOROMETHYL HYPOFLUORITE (CF3OF)
C1F8S1(G)                    PENTAFLUORO(TRIFLUOROMETHYL)SULFUR (CF3SF5)
C1H1(G)                      METHYLIDYNE (CH)
C1H1+(G)                     METHYLIDYNE, ION (CH+)
C1H1CL1(G)                   CHLOROMETHYLENE (CHCL)
C1H1CL1F2(G)                 CHLORODIFLUOROMETHANE (CHCLF2)
C1H1CL2F1(G)                 DICHLOROFLUOROMETHANE (CHCL2F)
C1H1CL3(G)                   TRICHLOROMETHANE (CHCL3)
C1H1F1(G)                    FLUOROMETHYLENE (CHF)
C1H1F1O1(G)                  FORMYL FLUORIDE (HCOF)
C1H1F3(G)                    TRIFLUOROMETHANE (CHF3)
C1H1N1(G)                    HYDROGEN CYANIDE (HCN)
C1H1N1O1(G)                  HYDROGEN ISOCYANATE (HNCO)
C1H1O1(G)                    FORMYL (HCO)
C1H1O1+(G)                   FORMYL, ION (HCO+)
C1H1P1(G)                    METHINOPHOSPHIDE (CHP)
C1H2(G)                      METHYLENE (CH2)
C1H2CL1F1(G)                 CHLOROFLUOROMETHANE (CH2CLF)
C1H2CL2(G)                   DICHLOROMETHANE (CH2CL2)
C1H2F2(G)                    DIFLUOROMETHANE (CH2F2)
C1H2O1(G)                    FORMALDEHYDE (H2CO)
C1H3(G)                      METHYL (CH3)
C1H3CL1(G)                   CHLOROMETHANE (CH3CL)
C1H3CL3SI1(G)                TRICHLOROMETHYLSILANE (SICH3CL3)
C1H3F1(G)                    FLUOROMETHANE (CH3F)
C1H3F3SI1(G)                 TRIFLUOROMETHYLSILANE (SICH3F3)
C1H4(G)                      METHANE (CH4)
C1I1N1(G)                    CYANOGEN IODIDE (CNI)
C1K1N1(CR)                   POTASSIUM CYANIDE (KCN)
C1K1N1(CR,L)                 POTASSIUM CYANIDE (KCN)
C1K1N1(G)                    POTASSIUM CYANIDE (KCN)
C1K1N1(L)                    POTASSIUM CYANIDE (KCN)
C1K2O3(CR)                   POTASSIUM CARBONATE (K2CO3)
C1K2O3(CR,L)                 POTASSIUM CARBONATE (K2CO3)
C1K2O3(L)                    POTASSIUM CARBONATE (K2CO3)
C1LI2O3(CR)                  LITHIUM CARBONATE (LI2CO3)
C1LI2O3(CR,L)                LITHIUM CARBONATE (LI2CO3)
C1LI2O3(L)                   LITHIUM CARBONATE (LI2CO3)
C1MG1O3(CR)                  MAGNESIUM CARBONATE (MGCO3)
C1NA2O3(CR)                  SODIUM CARBONATE (NA2CO3)
C1NA2O3(CR,L)                SODIUM CARBONATE (NACO3)
C1NA2O3(L)                   SODIUM CARBONATE (NA2CO3)
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C1N1(G)	CYANOGEN (CN)
C1N1+(G)	CYANOGEN, ION (CN+)
C1N1-(G)	CYANIDE (CN-)
C1N1NA1(CR)	SODIUM CYANIDE (NACN)
C1N1NA1(CR,L)	SODIUM CYANIDE (NACN)
C1N1NA1(G)	SODIUM CYANIDE (NACN)
C1N1NA1(L)	SODIUM CYANIDE (NACN)
C1N1O1(G)	NCO RADICAL (NC1O1)
C1N2(G)	CNN RADICAL (CNN)
C1N2(G)-B	NCN RADICAL (NCN)
C1O1(G)	CARBON MONOXIDE (CO)
C1O1S1(G)	CARBON OXIDE SULFIDE (COS)
C1O2(G)	CARBON DIOXIDE (CO2)
C1O2-(G)	CARBON DIOXIDE, ION (CO2-)
C1P1(G)	CARBON PHOSPHIDE (CP)
C1SI1(CR)	SILICON CARBIDE, ALPHA (SIC)
C1SI1(CR)-B	SILICON CARBIDE, BETA (SIC)
C1SI1(G)	SILICON CARBIDE (SIC)
C1SI2(G)	SILICON CARBIDE (SI2C)
C1S1(G)	CARBON SULFIDE (CS)
C1S2(G)	CARBON DISULFIDE (CS2)
C1TA1(CR)	TANTALUM CARBIDE (TAC)
C1TA1(CR,L)	TANTALUM CARBIDE (TAC)
C1TA1(L)	TANTALUM CARBIDE (TAC)
C1TI1(CR)	TITANIUM CARBIDE (TIC)
C1TI1(CR,L)	TITANIUM CARBIDE (TIC)
C1TI1(L)	TITANIUM CARBIDE (TIC)
C1ZR1(CR)	ZIRCONIUM CARBIDE (ZRC)
C1ZR1(CR,L)	ZIRCONIUM CARBIDE (ZRC)
C1ZR1(L)	ZIRCONIUM CARBIDE (ZRC)
C2(G)	CARBON (C2)
C2-(G)	CARBON, ION (C2-)
C2BE1(G)	BERYLLIUM CARBIDE (BEC2)
C2CL2(G)	DICHLOROETHYNE (C2CL2)
C2CL4(G)	TETRACHLOROETHENE (C2CL4)
C2CL6(G)	HEXACHLOROETHANE (C2CL6)
C2CR3(CR)	CHROMIUM CARBIDE (CR3C2)
C2F2(G)	DIFLUOROETHYNE (C2F2)
C2F3N1(G)	TRIFLUOROACETONITRILE (CF3CN)
C2F4(G)	TETRAFLUOROETHENE (C2F4)
C2F6(G)	HEXAFLUOROETHANE (C2F6)
C2H1(G)	ETHYNYL (C2H)
C2H1CL1(G)	CHLOROETHYNE (C2HCL)
C2H1F1(G)	FLUOROETHYNE (C2HF)
C2H2(G)	ETHYNE (C2H2)
C2H4(G)	ETHENE (C2H4)
C2H4O1(G)	OXIRANE (C2H4O)
C2K2N2(G)	POTASSIUM CYANIDE ((KCN)2)
C2LI2(CR)	LITHIUM CARBIDE (LI2C2)
C2MG1(CR)	MAGNESIUM CARBIDE (MGC2)
C2N1(G)	CNC RADICAL (C2N)
C2N2(G)	ETHANEDINITRILE ((CN)2)
C2N2NA2(G)	SODIUM CYANIDE ((NACN)2)
C2O1(G)	CCO RADICAL (C2O)

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C2SI1(G)              SILICON CARBIDE (SIC2)
C3(G)                 CARBON (C3)
C3AL4(CR)             ALUMINUM CARBIDE (AL4C3)
C3CR7(CR)             CHROMIUM CARBIDE (CR7C3)
C3MG2(CR)             MAGNESIUM CARBIDE (MG2C3)
C3O2(G)               CARBON SUBOXIDE (C3O2)
C4(G)                 CARBON (C4)
C4H12SI1(G)           TETRAMETHYLSILANE (SI(CH3)4)
C4NI1O4(G)            NICKEL CARBONYL (NI(CO)4)
C4NI1O4(L)            NICKEL CARBONYL (NI(CO)4)
C4N2(G)               2-BUTYNEDINITRILE (C4N2)
C5(G)                 CARBON (C5)
C5FE1O5(G)            IRON CARBONYL (FE(CO)5)
C5FE1O5(L)            IRON CARBONYL (FE(CO)5)
C6CR23(CR)            CHROMIUM CARBIDE (CR23C6)
D1(G)                 DEUTERIUM (D)
D1+(G)                DEUTERIUM, ION (D+)
D1-(G)                DEUTERIUM, ION (D-)
D1F1(G)               HYDROFLUORIC ACID-D (DF)
D1H1(G)               HYDROGEN-D1 (HD)
D1H1+(G)              HYDROGEN-D1, ION (HD+)
D1H1-(G)              HYDROGEN-D1, ION (HD-)
D1H1O1(G)             WATER-D1 (HDO)
D1N1(G)               IMIDOGEN-D1 (ND)
D1O1(G)               HYDROXYL-D1 (OD)
D1S1(G)               MERCAPTO-D1 (SD)
D2(REF)               DEUTERIUM (D2)
D2+(G)                DFUTERIUM, ION (D2+)
D2-(G)                DEUTERIUM, ION (D2-)
D2N1(G)               AMIDOGEN-D2 (ND2)
D2N2(G)               DIAZENE-D2, CIS (DNND)
D2O1(G)               WATER-D2 (D2O)
D2S1(G)               HYDROGEN SULFIDE-D2 (D2S)
D3N1(G)               AMMONIA-D3 (ND3)
E1-(REF)              ELECTRON GAS (E-)
FE0.877S1(CR)         IRON SULFIDE, PYRRHOTITE (FE0.877S)
FE0.947O1(CR)         IRON OXIDE, WUSTITE (FE0.947O)
FE1(CR)               IRON, ALPHA-DELTA (FE)
FE1(CR)-B             IRON, GAMMA (FE)
FE1(CR,L)             IRON (FE)
FE1(G)                IRON (FE)
FE1(L)                IRON (FE)
FE1(REF)              IRON (FE)
FE1+(G)               IRON, ION (FE+)
FE1-(G)               IRON, ION (FE-)
FE1H2O2(CR)           IRON HYDROXIDE (FE(OH)2)
FE1H2O2(G)            IRON HYDROXIDE (FE(OH)2)
FE1H3O3(CR)           IRON HYDROXIDE (FE(OH)3)
FE1I2(CR)             IRON IODIDE (FEI2)
FE1I2(CR,L)           IRON IODIDE (FEI2)
FE1I2(G)              IRON IODIDE (FEI2)
FE1I2(L)              IRON IODIDE (FEI2)
FE1O1(CR)             IRON OXIDE (FEO)
FE1O1(CR,L)           IRON OXIDE (FEO)
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FE1O1(G)	IRON OXIDE (FEO)
FE1O1(L)	IRON OXIDE (FEO)
FE1O4S1(CR)	IRON SULFATE (FESO4)
FE1S1(CR)	IRON SULFIDE, TROILITE (FES)
FE1S1(CR,L)	IRON SULFIDE, TROILITE (FES)
FE1S1(G)	IRON SULFIDE (FES)
FE1S1(L)	IRON SULFIDE (FES)
FE1S2(CR)	IRON SULFIDE, MARCASITE (FES2)
FE1S2(CR)-B	IRON SULFIDE, PYRITE (FES2)
FE2I4(G)	IRON IODIDE ((FEI2)2)
FE2O12S3(CR)	IRON SULFATE (FE2(SO4)3)
FE2O3(CR)	IRON OXIDE, HEMATITE (FE2O3)
FE3O4(CR)	IRON OXIDE, MAGNETITE (FE3O4)
F1(G)	FLUORINE (F)
F1+(G)	FLUORINE, ION (F+)
F1-(G)	FLUORINE, ION (F-)
F1FE1(G)	IRON FLUORIDE (FEF)
F1HG1(G)	MERCURY FLUORIDE (HGF)
F1H1(G)	HYDROGEN FLUORIDE (HF)
F1H1O1(G)	HYPOFLUOROUS ACID (HOF)
F1H1O3S1(G)	FLUOROSULFURIC ACID (HSO3F)
F1H3SI1(G)	FLUOROSILANE (SIH3F)
F1I1(G)	IODINE FLUORIDE (IF)
F1K1(CR)	POTASSIUM FLUORIDE (KF)
F1K1(CR,L)	POTASSIUM FLUORIDE (KF)
F1K1(G)	POTASSIUM FLUORIDE (KF)
F1K1(L)	POTASSIUM FLUORIDE (KF)
F1LI1(CR)	LITHIUM FLUORIDE (LIF)
F1LI1(CR,L)	LITHIUM FLUORIDE (LIF)
F1LI1(G)	LITHIUM FLUORIDE (LIF)
F1LI1(L)	LITHIUM FLUORIDE (LIF)
F1LI1O1(G)	LITHIUM HYPOFLUORITE (LIOF)
F1MG1(G)	MAGNESIUM FLUORIDE (MGF)
F1MG1+(G)	MAGNESIUM FLUORIDE, ION (MGF+)
F1MO1(G)	MOLYBDENUM FLUORIDE (MOF)
F1NA1(CR)	SODIUM FLUORIDE (NAF)
F1NA1(CR,L)	SODIUM FLUORIDE (NAF)
F1NA1(G)	SODIUM FLUORIDE (NAF)
F1NA1(L)	SODIUM FLUORIDE (NAF)
F1N1(G)	FLUOROIMIDOGEN (NF)
F1N1O1(G)	NITROSYL FLUORIDE (ONF)
F1N1O2(G)	NITRYL FLUORIDE (NO2F)
F1N1O3(G)	FLUORINE NITRATE (FONO2)
F1O1(G)	OXYGEN FLUORIDE (OF)
F1O1TI1(G)	TITANIUM FLUORIDE OXIDE (OTIF)
F1O2(G)	OXYGEN FLUORIDE (O2F)
F1PB1(G)	LEAD FLUORIDE (PBF)
F1P1(G)	PHOSPHORUS FLUORIDE (PF)
F1P1+(G)	PHOSPHORUS FLUORIDE, ION (PF+)
F1P1-(G)	PHOSPHORUS FLUORIDE, ION (PF-)
F1P1S1(G)	THIOPHOSPHORYL FLUORIDE (PSF)
F1SI1(G)	FLUOROSILYLIDYNE (SIF)
F1SR1(G)	STRONTIUM FLUORIDE (SRF)
F1SR1+(G)	STRONTIUM FLUORIDE, ION (SRF+)

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F1S1(G)            SULFUR FLUORIDE (SF)
F1S1+(G)           SULFUR FLUORIDE, ION (SF+)
F1S1-(G)           SULFUR FLUORIDE, ION (SF-)
F1TI1(G)           TITANIUM FLUORIDE (TIF)
F1W1(G)            TUNGSTEN FLUORIDE (WF)
F1ZR1(G)           ZIRCONIUM FLUORIDE (ZRF)
F10MO2(G)          MOLYBDENUM FLUORIDE ((MOF5)2)
F10S2(G)           SULFUR FLUORIDE (S2F10)
F15MO3(G)          MOLYBDENUM FLUORIDE ((MOF5)3)
F2(REF)            FLUORINE (F2)
F2FE1(CR)          IRON FLUORIDE (FEF2)
F2FE1(CR,L)        IRON FLUORIDE (FEF2)
F2FE1(G)           IRON FLUORIDE (FEF2)
F2FE1(L)           IRON FLUORIDE (FEF2)
F2HG1(CR)          MERCURY FLUORIDE (HGF2)
F2HG1(CR,L)        MERCURY FLUORIDE (HGF2)
F2HG1(G)           MERCURY FLUORIDE (HGF2)
F2HG1(L)           MERCURY FLUORIDE (HGF2)
F2HG2(CR)          MERCURY FLUORIDE (HG2F2)
F2H1K1(CR)         POTASSIUM FLUORIDE (K(HF2))
F2H1K1(CR,L)       POTASSIUM FLUORIDE (K(HF2))
F2H1K1(L)          POTASSIUM FLUORIDE (K(HF2))
F2H2(G)            HYDROGEN FLUORIDE ((HF)2)
F2H2SI1(G)         DIFLUOROSILANE (SIH2F2)
F2K1-(G)           POTASSIUM FLUORIDE, ION (KF2-)
F2K2(G)            POTASSIUM FLUORIDE ((KF)2)
F2LI1-(G)          LITHIUM FLUORIDE, ION (LIF2-)
F2LI2(G)           LITHIUM FLUORIDE ((LIF)2)
F2MG1(CR)          MAGNESIUM FLUORIDE (MGF2)
F2MG1(CR,L)        MAGNESIUM FLUORIDE (MGF2)
F2MG1(G)           MAGNESIUM FLUORIDE (MGF2)
F2MG1(L)           MAGNESIUM FLUORIDE (MGF2)
F2MG1+(G)          MAGNESIUM FLUORIDE, ION (MGF2+)
F2MO1(G)           MOLYBDENUM FLUORIDE (MOF2)
F2NA1-(G)          SODIUM FLUORIDE, ION (NAF2-)
F2NA2(G)           SODIUM FLUORIDE ((NAF)2)
F2N1(G)            DIFLUOROAMIDOGEN (NF2)
F2N2(G)            NITROGEN FLUORIDE, CIS (FNNF)
F2N2(G)-B          NITROGEN FLUORIDE, TRANS (FNNF)
F2O1(G)            OXYGEN FLUORIDE (OF2)
F2O1SI1(G)         DIFLUOROOXOSILANE (OSIF2)
F2O1S1(G)          THIONYL FLUORIDE (OSF2)
F2O1TI1(G)         TITANIUM FLUORIDE OXIDE (OTIF2)
F2O2S1(G)          SULFURYL FLUORIDE (SO2F2)
F2PB1(CR)          LEAD FLUORIDE, ALPHA (PBF2)
F2PB1(CR)-B        LEAD FLUORIDE, BETA (PBF2)
F2PB1(CR,L)        LEAD FLUORIDE (PBF2)
F2PB1(G)           LEAD FLUORIDE (PBF2)
F2PB1(L)           LEAD FLUORIDE (PBF2)
F2P1(G)            PHOSPHORUS FLUORIDE (PF2)
F2P1+(G)           PHOSPHORUS FLUORIDE, ION (PF2+)
F2P1-(G)           PHOSPHORUS FLUORIDE, ION (PF2-)
F2SI1(G)           DIFLUOROSILYLENE (SIF2)
F2SR1(CR)          STRONTIUM FLUORIDE (SRF2)
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F2SR1(CR,L)	STRONTIUM FLUORIDE (SRF2)
F2SR1(G)	STRONTIUM FLUORIDE (SRF2)
F2SR1(L)	STRONTIUM FLUORIDE (SRF2)
F2S1(G)	SULFUR FLUORIDE (SF2)
F2S1+(G)	SULFUR FLUORIDE, ION (SF2+)
F2S1-(G)	SULFUR FLUORIDE, ION (SF2-)
F2S2(G)	DIFLUORODISULFANE (FSSF)
F2S2(G)-B	THIOTHIONYL FLUORIDE (SSF2)
F2TI1(G)	TITANIUM FLUORIDE (TIF2)
F2ZR1(CR)	ZIRCONIUM FLUORIDE (ZRF2)
F2ZR1(CR,L)	ZIRCONIUM FLUORIDE (ZRF2)
F2ZR1(G)	ZIRCONIUM FLUORIDE (ZRF2)
F2ZR1(L)	ZIRCONIUM FLUORIDE (ZRF2)
F3FE1(CR)	IRON FLUORIDE (FEF3)
F3FE1(G)	IRON FLUORIDE (FEF3)
F3H1SI1(G)	TRIFLUOROSILANE (SIHF3)
F3H3(G)	HYDROGEN FLUORIDE (H3F3)
F3LI3(G)	LITHIUM FLUORIDE ((LIF)3)
F3MO1(G)	MOLYBDENUM FLUORIDE (MOF3)
F3N1(G)	NITROGEN FLUORIDE (NF3)
F3N1O1(G)	NITROGEN FLUORIDE OXIDE (NF3O)
F3O1P1(G)	PHOSPHORYL FLUORIDE (POF3)
F3P1(G)	PHOSPHORUS FLUORIDE (PF3)
F3P1S1(G)	THIOPHOSPHORYL FLUORIDE (PSF3)
F3SI1(G)	TRIFLUOROSILYL (SIF3)
F3S1(G)	SULFUR FLUORIDE (SF3)
F3S1+(G)	SULFUR FLUORIDE, ION (SF3+)
F3S1-(G)	SULFUR FLUORIDE, ION (SF3-)
F3TI1(CR)	TITANIUM FLUORIDE (TIF3)
F3TI1(G)	TITANIUM FLUORIDE (TIF3)
F3ZR1(CR)	ZIRCONIUM FLUORIDE (ZRF3)
F3ZR1(G)	ZIRCONIUM FLUORIDE (ZRF3)
F4H4(G)	HYDROGEN FLUORIDE (H4F4)
F4MG2(G)	MAGNESIUM FLUORIDE ((MGF2)2)
F4MO1(G)	MOLYBDENUM FLUORIDE (MOF4)
F4MO1O1(G)	MOLYBDENUM FLUORIDE OXIDE (MOF4O)
F4N2(G)	TETRAFLUOROHYDRAZINE (N2F4)
F4O1W1(CR)	TUNGSTEN FLUORIDE OXIDE (WF4O)
F4O1W1(CR,L)	TUNGSTEN FLUORIDE OXIDE (WF4O)
F4O1W1(G)	TUNGSTEN FLUORIDE OXIDE (WF4O)
F4O1W1(L)	TUNGSTEN FLUORIDE OXIDE (WF4O)
F4PB1(G)	LEAD FLUORIDE (PBF4)
F4SI1(G)	TETRAFLUOROSILANE (SIF4)
F4S1(G)	SULFUR FLUORIDE (SF4)
F4S1+(G)	SULFUR FLUORIDE, ION (SF4+)
F4S1-(G)	SULFUR FLUORIDE, ION (SF4-)
F4TI1(CR)	TITANIUM FLUORIDE (TIF4)
F4TI1(G)	TITANIUM FLUORIDE (TIF4)
F4ZR1(CR)	ZIRCONIUM FLUORIDE (ZRF4)
F4ZR1(G)	ZIRCONIUM FLUORIDE (ZRF4)
F5H5(G)	HYDROGEN FLUORIDE (H5F5)
F5I1(G)	IODINE FLUORIDE (IF5)
F5MO1(G)	MOLYBDENUM FLUORIDE (MOF5)
F5P1(G)	PHOSPHORUS FLUORIDE (PF5)

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F5S1(G)              SULFUR FLUORIDE (SF5)
F5S1+(G)             SULFUR FLUORIDE, ION (SF5+)
F5S1-(G)             SULFUR FLUORIDE, ION (SF5-)
F6H6(G)              HYDROGEN FLUORIDE (H6F6)
F6MO1(G)             MOLYBDENUM FLUORIDE (MOF6)
F6MO1(L)             MOLYBDENUM FLUORIDE (MOF6)
F6S1(G)              SULFUR FLUORIDE (SF6)
F6S1-(G)             SULFUR FLUORIDE, ION (SF6-)
F6W1(G)              TUNGSTEN FLUORIDE (WF6)
F6W1(L)              TUNGSTEN FLUORIDE (WF6)
F7H7(G)              HYDROGEN FLUORIDE (H7F7)
F7I1(G)              IODINE FLUORIDE (IF7)
GA1(CR)              GALLIUM (GA)
GA1(CR,L)            GALLIUM (GA)
GA1(G)               GALLIUM (GA)
GA1(L)               GALLIUM (GA)
GA1(REF)             GALLIUM (GA)
GA1+(G)              GALLIUM, ION (GA+)
GA1-(G)              GALLIUM, ION  (GA-)
HE1(REF)             HELIUM (HE)
HE1+(G)              HELIUM, ION (HE+)
HF1(CR)              HAFNIUM, ALPHA (HF)
HF1(CR)-B            HAFNIUM, BETA (HF)
HF1(CR,L)            HAFNIUM (HF)
HF1(G)               HAFNIUM (HF)
HF1(L)               HAFNIUM (HF)
HF1(REF)             HAFNIUM (HF)
HF1+(G)              HAFNIUM, ION (HF+)
HF1-(G)              HAFNIUM, ION (HF-)
HG1(CR,L)            MERCURY (HG)
HG1(G)               MERCURY (HG)
HG1(REF)             MERCURY (HG)
HG1+(G)              MERCURY, ION (HG+)
HG1I1(G)             MERCURY IODIDE (HGI)
HG1I2(CR)            MERCURY IODIDE (HGI2)
HG1I2(CR,L)          MERCURY IODIDE (HGI2)
HG1I2(G)             MERCURY IODIDE (HGI2)
HG1I2(L)             MERCURY IODIDE (HGI2)
HG1O1(CR)            MERCURY OXIDE (HGO)
HG1O1(G)             MERCURY OXIDE (HGO)
HG2I2(CR)            MERCURY IODIDE (HG2I2)
HG2I2(CR,L)          MERCURY IODIDE (HG2I2)
HG2I2(L)             MERCURY IODIDE (HG2I2)
H1(G)                HYDROGEN (H)
H1+(G)               HYDROGEN, ION (H+)
H1-(G)               HYDROGEN, ION (H-)
H1HG1(G)             MERCURY HYDRIDE (HGH)
H1I1(G)              HYDROGEN IODIDE (HI)
H1I3SI1(G)           TRIIODOSILANE (SIHI3)
H1K1(CR)             POTASSIUM HYDRIDE (KH)
H1K1(G)              POTASSIUM HYDRIDE (KH)
H1K1O1(CR)           POTASSIUM HYDROXIDE (KOH)
H1K1O1(CR,L)         POTASSIUM HYDROXIDE (KOH)
H1K1O1(G)            POTASSIUM HYDROXIDE (KOH)
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H1K1O1(L)	POTASSIUM HYDROXIDE (KOH)
H1K1O1+(G)	POTASSIUM HYDROXIDE, ION (KOH+)
H1LI1(CR)	LITHIUM HYDRIDE (LIH)
H1LI1(CR,L)	LITHIUM HYDRIDE (LIH)
H1LI1(G)	LITHIUM HYDRIDE (LIH)
H1LI1(L)	LITHIUM HYDRIDE (LIH)
H1LI1O1(CR)	LITHIUM HYDROXIDE (LIOH)
H1LI1O1(CR,L)	LITHIUM HYDROXIDE (LIOH)
H1LI1O1(G)	LITHIUM HYDROXIDE (LIOH)
H1LI1O1(L)	LITHIUM HYDROXIDE (LIOH)
H1LI1O1+(G)	LITHIUM HYDROXIDE, ION (LIOH+)
H1MG1(G)	MAGNESIUM HYDRIDE (MGH)
H1MG1O1(G)	MAGNESIUM HYDROXIDE (MGOH)
H1MG1O1+(G)	MAGNESIUM HYDROXIDE, ION (MGOH+)
H1NA1(CR)	SODIUM HYDRIDE (NAH)
H1NA1(G)	SODIUM HYDRIDE (NAH)
H1NA1O1(CR)	SODIUM HYDROXIDE (NAOH)
H1NA1O1(CR,L)	SODIUM HYDROXIDE (NAOH)
H1NA1O1(G)	SODIUM HYDROXIDE (NAOH)
H1NA1O1(L)	SODIUM HYDROXIDE (NAOH)
H1NA1O1+(G)	SODIUM HYDROXIDE, ION (NAOH+)
H1N1(G)	IMIDOGEN (NH)
H1N1O1(G)	NITROSYL HYDRIDE (HNO)
H1N1O2(G)	NITROUS ACID, CIS (HONO)
H1N1O2(G)-B	NITROUS ACID, TRANS (HONO)
H1N1O3(G)	NITRIC ACID (HONO2)
H1O1(G)	HYDROXYL (OH)
H1O1+(G)	HYDROXYL, ION (OH+)
H1O1-(G)	HYDROXYL, ION (OH-)
H1O1SR1(G)	STRONTIUM HYDROXIDE (SROH)
H1O1SR1+(G)	STRONTIUM HYDROXIDE, ION (SROH+)
H1O2(G)	HYDROPEROXO (HOO)
H1PB1(G)	LEAD HYDRIDE (PBH)
H1P1(G)	PHOSPHINIDENE (PH)
H1SI1(G)	SILYLIDYNE (SIH)
H1SI1+(G)	SILYLIDYNE, ION (SIH+)
H1S1(G)	MERCAPTO (HS)
H1ZR1(G)	ZIRCONIUM HYDRIDE (ZRH)
H10O8S1(CR,L)	SULFURIC ACID, TETRAHYDRATE (H2SO4.4H2O)
H15O10.5S1(CR,L)	SULFURIC ACID, HEMIHEXAHYDRATE (H2SO4.6.5H2O
H2(REF)	HYDROGEN (H2)
H2+(G)	HYDROGEN, ION (H2+)
H2-(G)	HYDROGEN, ION (H2-)
H2I2SI1(G)	DIIODOSILANE (SIH2I2)
H2K2O2(G)	POTASSIUM HYDROXIDE ((KOH)2)
H2LI2O2(G)	LITHIUM HYDROXIDE ((LIOH)2)
H2MG1(CR)	MAGNESIUM HYDRIDE (MGH2)
H2MG1O2(CR)	MAGNESIUM HYDROXIDE (MG(OH)2)
H2MG1O2(G)	MAGNESIUM HYDROXIDE (MG(OH)2)
H2MO1O4(G)	MOLYBDIC ACID (O2MO(OH)2)
H2NA2O2(G)	SODIUM HYDROXIDE ((NAOH)2)
H2N1(G)	AMIDOGEN (NH2)
H2N2(G)	DIAZENE, CIS (HNNH)
H2O1(FL)	WATER, 500 BAR (H2O)

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H2O1(FL)-B              WATER, 5000 BAR (H2O)
H2O1(G)                 WATER (H2O)
H2O1(L)                 WATER (H2O)
H2O1(L,G)               WATER, 1 BAR (H2O)
H2O1(L,G)-B             WATER, 10 BAR (H2O)
H2O1(L,G)-C             WATER, 100 BAR (H2O)
H2O2(G)                 HYDROGEN PEROXIDE (HOOH)
H2O2SR1(CR)             STRONTIUM HYDROXIDE (SR(OH)2)
H2O2SR1(CR,L)           STRONTIUM HYDROXIDE (SR(OH)2)
H2O2SR1(G)              STRONTIUM HYDROXIDE (SR(OH)2)
H2O2SR1(L)              STRONTIUM HYDROXIDE (SR(OH)2)
H2O4S1(CR,L)            SULFURIC ACID (O2S(OH)2)
H2O4S1(G)               SULFURIC ACID (O2S(OH)2)
H2O4W1(CR)              TUNGSTIC ACID (O2W(OH)2)
H2O4W1(G)               TUNGSTIC ACID (O2W(OH)2)
H2P1(G)                 PHOSPHINO (PH2)
H2S1(G)                 HYDROGEN SULFIDE (H2S)
H2TI1(CR)               TITANIUM HYDRIDE (TIH2)
H3I1SI1(G)              IODOSILANE (SIH3I)
H3N1(G)                 AMMONIA (NH3)
H3O1+(G)                HYDRONIUM, ION (H3O+)
H3O4P1(CR)              PHOSPHORIC ACID (H3PO4)
H3O4P1(CR,L)            PHOSPHORIC ACID (H3PO4)
H3O4P1(L)               PHOSPHORIC ACID (H3PO4)
H3P1(G)                 PHOSPHINE (PH3)
H4I1N1(CR)              AMMONIUM IODIDE (NH4I)
H4N2(G)                 HYDRAZINE (N2H4)
H4N2(L)                 HYDRAZINE (N2H4)
H4O5S1(CR,L)            SULFURIC ACID, MONOHYDRATE (H2SO4.H2O)
H4SI1(G)                SILANE (SIH4)
H6O6S1(CR,L)            SULFURIC ACID, DIHYDRATE (H2SO4.2H2O)
H8O7S1(CR,L)            SULFURIC ACID, TRIHYDRATE (H2SO4.3H2O)
I1(G)                   IODINE (I)
I1+(G)                  IODINE, ION (I+)
I1-(G)                  IODINE, ION (I-)
I1K1(CR)                POTASSIUM IODIDE (KI)
I1K1(CR,L)              POTASSIUM IODIDE (KI)
I1K1(G)                 POTASSIUM IODIDE (KI)
I1K1(L)                 POTASSIUM IODIDE (KI)
I1LI1(CR)               LITHIUM IODIDE (LII)
I1LI1(CR,L)             LITHIUM IODIDE (LII)
I1LI1(G)                LITHIUM IODIDE (LII)
I1LI1(L)                LITHIUM IODIDE (LII)
I1MG1(G)                MAGNESIUM IODIDE (MGI)
I1MO1(G)                MOLYBDENUM IODIDE (MOI)
I1NA1(CR)               SODIUM IODIDE (NAI)
I1NA1(CR,L)             SODIUM IODIDE (NAI)
I1NA1(L)                SODIUM IODIDE (NAI)
I1N1O1(G)               NITROSYL IODIDE (ONI)
I1PB1(G)                LEAD IODIDE (PBI)
I1SI1(G)                IODOSILYLIDYNE (SII)
I1SR1(G)                STRONTIUM IODIDE (SRI)
I1TI1(G)                TITANIUM IODIDE (TII)
I1ZR1(G)                ZIRCONIUM IODIDE (ZRI)
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I2(CR)	IODINE (I2)
I2(CR,L)	IODINE (I2)
I2(G)	IODINE (I2)
I2(L)	IODINE (I2)
I2(REF)	IODINE (I2)
I2K2(G)	POTASSIUM IODIDE ((KI)2)
I2LI2(G)	LITHIUM IODIDE ((LII)2)
I2MG1(CR)	MAGNESIUM IODIDE (MGI2)
I2MG1(CR,L)	MAGNESIUM IODIDE (MGI2)
I2MG1(G)	MAGNESIUM IODIDE (MGI2)
I2MG1(L)	MAGNESIUM IODIDE (MGI2)
I2MO1(CR)	MOLYBDENUM IODIDE, ALPHA (MOI2)
I2MO1(G)	MOLYBDENUM IODIDE (MOI2)
I2PB1(CR)	LEAD IODIDE (PBI2)
I2PB1(CR,L)	LEAD IODIDE (PBI2)
I2PB1(G)	LEAD IODIDE (PBI2)
I2PB1(L)	LEAD IODIDE (PBI2)
I2SI1(G)	DIIODOSILYLENE (SII2)
I2SR1(CR)	STRONTIUM IODIDE (SRI2)
I2SR1(CR,L)	STRONTIUM IODIDE (SRI2)
I2SR1(G)	STRONTIUM IODIDE (SRI2)
I2SR1(L)	STRONTIUM IODIDE (SRI2)
I2TI1(CR)	TITANIUM IODIDE (TII2)
I2TI1(G)	TITANIUM IODIDE (TII2)
I2ZR1(CR)	ZIRCONIUM IODIDE (ZRI2)
I2ZR1(CR,L)	ZIRCONIUM IODIDE (ZRI2)
I2ZR1(G)	ZIRCONIUM IODIDE (ZRI2)
I2ZR1(L)	ZIRCONIUM IODIDE (ZRI2)
I3MO1(CR)	MOLYBDENUM IODIDE (MOI3)
I3MO1(G)	MOLYBDENUM IODIDE (MOI3)
I3SI1(G)	TRIIODOSILYL (SII3)
I3TI1(CR)	TITANIUM IODIDE (TII3)
I3TI1(G)	TITANIUM IODIDE (TII3)
I3ZR1(CR)	ZIRCONIUM IODIDE (ZRI3)
I3ZR1(G)	ZIRCONIUM IODIDE (ZRI3)
I4MO1(CR)	MOLYBDENUM IODIDE (MOI4)
I4MO1(G)	MOLYBDENUM IODIDE (MOI4)
I4PB1(G)	LEAD IODIDE (PBI4)
I4SI1(CR)	TETRAIODOSILANE (SII4)
I4SI1(CR,L)	TETRAIODOSILANE (SII4)
I4SI1(G)	TETRAIODOSILANE (SII4)
I4SI1(L)	TETRAIODOSILANE (SII4)
I4TI1(CR)	TITANIUM IODIDE (TII4)
I4TI1(CR,L)	TITANIUM IODIDE (TII4)
I4TI1(G)	TITANIUM IODIDE (TII4)
I4TI1(L)	TITANIUM IODIDE (TII4)
I4ZR1(CR)	ZIRCONIUM IODIDE (ZRI4)
I4ZR1(G)	ZIRCONIUM IODIDE (ZRI4)
KR1(REF)	KRYPTON (KR)
KR1+(G)	KRYPTON, ION (KR+)
K1(CR)	POTASSIUM (K)
K1(CR,L)	POTASSIUM (K)
K1(G)	POTASSIUM (K)
K1(L)	POTASSIUM (K)

K1(REF)	POTASSIUM (K)
K1+(G)	POTASSIUM, ION (K+)
K1-(G)	POTASSIUM, ION (K-)
K1O1(G)	POTASSIUM OXIDE (KO)
K1O1-(G)	POTASSIUM OXIDE, ION (KO-)
K1O2(CR)	POTASSIUM SUPEROXIDE (KO2)
K2(G)	POTASSIUM (K2)
K2O1(CR)	POTASSIUM OXIDE (K2O)
K2O2(CR)	POTASSIUM PEROXIDE (K2O2)
K2O3SI1(CR)	POTASSIUM SILICATE (K2SIO3)
K2O3SI1(CR,L)	POTASSIUM SILICATE (K2SIO3)
K2O3SI1(L)	POTASSIUM SILICATE (K2SIO3)
K2O4S1(CR)	POTASSIUM SULFATE, ALPHA (K2SO4)
K2O4S1(CR)-B	POTASSIUM SULFATE, BETA (K2SO4)
K2O4S1(CR,L)	POTASSIUM SULFATE (K2SO4)
K2O4S1(G)	POTASSIUM SULFATE (K2SO4)
K2O4S1(L)	POTASSIUM SULFATE (K2SO4)
K2S1(CR)	POTASSIUM SULFIDE (K2S)
K2S1(CR,L)	POTASSIUM SULFIDE (K2S)
K2S1(L)	POTASSIUM SULFIDE (K2S)
LI1(CR)	LITHIUM (LI)
LI1(CR,L)	LITHIUM (LI)
LI1(G)	LITHIUM (LI)
LI1(L)	LITHIUM (LI)
LI1(REF)	LITHIUM (LI)
LI1+(G)	LITHIUM, ION (LI+)
LI1-(G)	LITHIUM, ION (LI-)
LI1NA1O1(G)	LITHIUM SODIUM OXIDE (LIONA)
LI1N1(G)	LITHIUM NITRIDE (LIN)
LI1N1O1(G)	LITHIUM OXYNITRIDE (LION)
LI1O1(G)	LITHIUM OXIDE (LIO)
LI1O1-(G)	LITHIUM OXIDE, ION (LIO-)
LI2(G)	LITHIUM (LI2)
LI2O1(CR)	LITHIUM OXIDE (LI2O)
LI2O1(CR,L)	LITHIUM OXIDE (LI2O)
LI2O1(G)	LITHIUM OXIDE (LI2O)
LI2O1(L)	LITHIUM OXIDE (LI2O)
LI2O2(CR)	LITHIUM PEROXIDE (LI2O2)
LI2O2(G)	LITHIUM OXIDE ((LIO)2)
LI2O3SI1(CR)	LITHIUM SILICATE (LI2SIO3)
LI2O3SI1(CR,L)	LITHIUM SILICATE (LI2SIO3)
LI2O3SI1(L)	LITHIUM SILICATE (LI2SIO3)
LI2O3TI1(CR)	LITHIUM TITANIUM OXIDE (LI2TIO3)
LI2O3TI1(CR,L)	LITHIUM TITANIUM OXIDE (LI2TIO3)
LI2O3TI1(L)	LITHIUM TITANIUM OXIDE (LI2TIO3)
LI2O4S1(CR)	LITHIUM SULFATE, ALPHA (LI2SO4)
LI2O4S1(CR)-B	LITHIUM SULFATE, BETA (LI2SO4)
LI2O4S1(CR,L)	LITHIUM SULFATE (LI2SO4)
LI2O4S1(G)	LITHIUM SULFATE (LI2SO4)
LI2O4S1(L)	LITHIUM SULFATE (LI2SO4)
LI2O5SI2(CR)	LITHIUM SILICATE (LI2SI2O5)
LI2O5SI2(CR,L)	LITHIUM SILICATE (LI2SI2O5)
LI2O5SI2(L)	LITHIUM SILICATE (LI2SI2O5)
LI3N1(CR)	LITHIUM NITRIDE (LI3N)

MG1(CR)	MAGNESIUM (MG)
MG1(CR,L)	MAGNESIUM (MG)
MG1(G)	MAGNESIUM (MG)
MG1(L)	MAGNESIUM (MG)
MG1(REF)	MAGNESIUM (MG)
MG1+(G)	MAGNESIUM, ION (MG+)
MG1N1(G)	MAGNESIUM NITRIDE (MGN)
MG1O1(CR)	MAGNESIUM OXIDE (MGO)
MG1O1(CR,L)	MAGNESIUM OXIDE (MGO)
MG1O1(G)	MAGNESIUM OXIDE (MGO)
MG1O1(L)	MAGNESIUM OXIDE (MGO)
MG1O3SI1(CR)	MAGNESIUM SILICATE (MGSIO3)
MG1O3SI1(CR,L)	MAGNESIUM SILICATE (MGSIO3)
MG1O3SI1(L)	MAGNESIUM SILICATE (MGSIO3)
MG1O3TI1(CR)	MAGNESIUM TITANIUM OXIDE (MGTIO3)
MG1O3TI1(CR,L)	MAGNESIUM TITANIUM OXIDE (MGTIO3)
MG1O3TI1(L)	MAGNESIUM TITANIUM OXIDE (MGTIO3)
MG1O4S1(CR)	MAGNESIUM SULFATE (MGSO4)
MG1O4S1(CR,L)	MAGNESIUM SULFATE (MGSO4)
MG1O4S1(L)	MAGNESIUM SULFATE (MGSO4)
MG1O4W1(CR)	MAGNESIUM TUNGSTEN OXIDE (MGWO4)
MG1O5TI2(CR)	MAGNESIUM TITANIUM OXIDE (MGTI2O5)
MG1O5TI2(CR,L)	MAGNESIUM TITANIUM OXIDE (MGTI2O5)
MG1O5TI2(L)	MAGNESIUM TITANIUM OXIDE (MGTI2O5)
MG1S1(CR)	MAGNESIUM SULFIDE (MGS)
MG1S1(G)	MAGNESIUM SULFIDE (MGS)
MG2(G)	MAGNESIUM (MG2)
MG2O4SI1(CR)	MAGNESIUM SILICATE (MG2SIO4)
MG2O4SI1(CR,L)	MAGNESIUM SILICATE (MG2SIO4)
MG2O4SI1(L)	MAGNESIUM SILICATE (MG2SIO4)
MG2O4TI1(CR)	MAGNESIUM TITANIUM OXIDE (MG2TIO4)
MG2O4TI1(CR,L)	MAGNESIUM TITANIUM OXIDE (MG2TIO4)
MG2O4TI1(L)	MAGNESIUM TITANIUM OXIDE (MG2TIO4)
MG2SI1(CR)	MAGNESIUM SILICIDE (MG2SI)
MG2SI1(CR,L)	MAGNESIUM SILICIDE (MG2SI)
MG2SI1(L)	MAGNESIUM SILICIDE (MG2SI)
MG3N2(CR)	MAGNESIUM NITRIDE (MG3N2)
MG3O8P2(CR)	MAGNESIUM PHOSPHATE (MG3P2O8)
MG3O8P2(CR,L)	MAGNESIUM PHOSPHATE (MG3P2O8)
MG3O8P2(L)	MAGNESIUM PHOSPHATE (MG3P2O8)
MN1(CR)	MANGANESE (MN)
MN1(CR,L)	MANGANESE (MN)
MN1(G)	MANGANESE (MN)
MN1(L)	MANGANESE (MN)
MN1(REF)	MANGANESE (MN)
MN1+(G)	MANGANESE, ION (MN+)
MO1(CR)	MOLYBDENUM (MO)
MO1(CR,L)	MOLYBDENUM (MO)
MO1(G)	MOLYBDENUM (MO)
MO1(L)	MOLYBDENUM (MO)
MO1(REF)	MOLYBDENUM (MO)
MO1+(G)	MOLYBDENUM, ION (MO+)
MO1-(G)	MOLYBDENUM, ION (MO-)
MO1O1(G)	MOLYBDENUM OXIDE (MOO)

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MO1O2.750(CR)              MOLYBDENUM OXIDE (MOO2.750)
MO1O2.875(CR)              MOLYBDENUM OXIDE (MOO2.875)
MO1O2.889(CR)              MOLYBDENUM OXIDE (MOO2.889)
MO1O2(CR)                  MOLYBDENUM OXIDE (MOO2)
MO1O2(G)                   MOLYBDENUM OXIDE (MOO2)
MO1O3(CR)                  MOLYBDENUM OXIDE (MOO3)
MO1O3(CR,L)                MOLYBDENUM OXIDE (MOO3)
MO1O3(G)                   MOLYBDENUM OXIDE (MOO3)
MO1O3(L)                   MOLYBDENUM OXIDE (MOO3)
MO1S2(CR)                  MOLYBDENUM SULFIDE (MOS2)
MO2S3(CR)                  MOLYBDENUM SULFIDE (MO2S3)
MO2S3(CR,L)                MOLYBDENUM SULFIDE (MO2S3)
MO2S3(L)                   MOLYBDENUM SULFIDE (MO2S3)
NA1(CR)                    SODIUM (NA)
NA1(CR,L)                  SODIUM (NA)
NA1(G)                     SODIUM (NA)
NA1(L)                     SODIUM (NA)
NA1(REF)                   SODIUM (NA)
NA1+(G)                    SODIUM, ION (NA+)
NA1-(G)                    SODIUM, ION  (NA-)
NA1O1(G)                   SODIUM OXIDE (NAO)
NA1O1-(G)                  SODIUM OXIDE, ION (NAO-)
NA1O2(CR)                  SODIUM SUPEROXIDE (NAO2)
NA2(G)                     SODIUM (NA2)
NA2O1(CR)                  SODIUM OXIDE (NA2O)
NA2O1(CR,L)                SODIUM OXIDE (NA2O)
NA2O1(L)                   SODIUM OXIDE (NA2O)
NA2O2(CR)                  SODIUM PEROXIDE (NA2O2)
NA2O3SI1(CR)               SODIUM SILICATE (NA2SIO3)
NA2O3SI1(CR,L)             SODIUM SILICATE (NA2SIO3)
NA2O3SI1(L)                SODIUM SILICATE (NA2SIO3)
NA2O4S1(CR)                SODIUM SULFATE, DELTA (NA2SO4)
NA2O4S1(CR)-B              SODIUM SULFATE, I (NA2SO4)
NA2O4S1(CR)-C              SODIUM SULFATE, III (NA2SO4)
NA2O4S1(CR)-D              SODIUM SULFATE, IV (NA2SO4)
NA2O4S1(CR)-E              SODIUM SULFATE, V (NA2SO4)
NA2O4S1(CR,L)              SODIUM SULFATE (NA2SO4)
NA2O4S1(G)                 SODIUM SULFATE (NA2SO4)
NA2O4S1(L)                 SODIUM SULFATE (NA2SO4)
NA2O4W1(CR)                SODIUM TUNGSTEN OXIDE (NA2WO4)
NA2O5SI2(CR)               SODIUM SILICATE (NA2SI2O5)
NA2O5SI2(CR,L)             SODIUM SILICATE (NA2SI2O5)
NA2O5SI2(L)                SODIUM SILICATE (NA2SI2O5)
NA2S1(CR)                  SODIUM SULFIDE (NA2S)
NA2S1(CR,L)                SODIUM SULFIDE (NA2S)
NA2S1(L)                   SODIUM SULFIDE (NA2S)
NA2S2(CR)                  SODIUM SULFIDE, BETA (NA2S2)
NA2S2(CR,L)                SODIUM SULFIDE (NA2S2)
NA2S2(L)                   SODIUM SULFIDE (NA2S2)
NB1(CR)                    NIOBIUM (NB)
NB1(CR,L)                  NIOBIUM (NB)
NB1(G)                     NIOBIUM (NB)
NB1(L)                     NIOBIUM (NB)
NB1(REF)                   NIOBIUM (NB)
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NB1+(G)	NIOBIUM, ION (NB+)
NB1-(G)	NIOBIUM, ION (NB-)
NB1O1(CR)	NIOBIUM OXIDE (NBO)
NB1O1(CR,L)	NIOBIUM OXIDE (NBO)
NB1O1(G)	NIOBIUM OXIDE (NBO)
NB1O1(L)	NIOBIUM OXIDE (NBO)
NB1O2(CR)	NIOBIUM OXIDE (NBO2)
NB1O2(CR,L)	NIOBIUM OXIDE (NBO2)
NB1O2(G)	NIOBIUM OXIDE (NBO2)
NB1O2(L)	NIOBIUM OXIDE (NBO2)
NB2O5(CR)	NIOBIUM OXIDE (NB2O5)
NB2O5(CR,L)	NIOBIUM OXIDE (NB2O5)
NB2O5(L)	NIOBIUM OXIDE (NB2O5)
NE1(REF)	NEON (NE)
NE1+(G)	NEON, ION (NE+)
NI1(CR)	NICKEL (NI)
NI1(CR,L)	NICKEL (NI)
NI1(G)	NICKEL (NI)
NI1(L)	NICKEL (NI)
NI1(REF)	NICKEL (NI)
NI1+(G)	NICKEL, ION (NI+)
NI1-(G)	NICKEL, ION (NI-)
NI1S1(CR)	NICKEL SULFIDE (NIS)
NI1S1(CR,L)	NICKEL SULFIDE (NIS)
NI1S1(G)	NICKEL SULFIDE (NIS)
NI1S1(L)	NICKEL SULFIDE (NIS)
NI1S2(CR)	NICKEL SULFIDE (NIS2)
NI1S2(CR,L)	NICKEL SULFIDE (NIS2)
NI1S2(L)	NICKEL SULFIDE (NIS2)
NI3S2(CR)	NICKEL SULFIDE (NI3S2)
NI3S2(CR,L)	NICKEL SULFIDE (NI3S2)
NI3S2(L)	NICKEL SULFIDE (NI3S2)
NI3S4(CR)	NICKEL SULFIDE (NI3S4)
N0.465V1(CR)	VANADIUM NITRIDE (VN0.465)
N1(G)	NITROGEN (N)
N1+(G)	NITROGEN, ION (N+)
N1-(G)	NITROGEN, ION (N-)
N1O1(G)	NITROGEN OXIDE (NO)
N1O1+(G)	NITROGEN OXIDE, ION (NO+)
N1O2(G)	NITROGEN OXIDE (NO2)
N1O2-(G)	NITROGEN OXIDE, ION (ONO-)
N1O3(G)	NITROGEN OXIDE (NO3)
N1P1(G)	PHOSPHORUS NITRIDE (PN)
N1SI1(G)	SILICON NITRIDE (SIN)
N1SI2(G)	SILICON NITRIDE (SI2N)
N1S1(G)	NITROGEN SULFIDE (NS)
N1TI1(CR)	TITANIUM NITRIDE (TIN)
N1TI1(CR,L)	TITANIUM NITRIDE (TIN)
N1TI1(L)	TITANIUM NITRIDE (TIN)
N1V1(CR)	VANADIUM NITRIDE (VN)
N1V1(G)	VANADIUM NITRIDE (VN)
N1ZR1(CR)	ZIRCONIUM NITRIDE (ZRN)
N1ZR1(CR,L)	ZIRCONIUM NITRIDE (ZRN)
N1ZR1(G)	ZIRCONIUM NITRIDE (ZRN)

N1ZR1(L)	ZIRCONIUM NITRIDE (ZRN)
N2(REF)	NITROGEN (N2)
N2+(G)	NITROGEN, ION (N2+)
N2-(G)	NITROGEN, ION (N2-)
N2O1(G)	NITROGEN OXIDE (N2O)
N2O1+(G)	NITROGEN OXIDE, ION (N2O+)
N2O3(G)	NITROGEN OXIDE (N2O3)
N2O4(CR)	NITROGEN OXIDE (N2O4)
N2O4(CR,L)	NITROGEN OXIDE (N2O4)
N2O4(G)	NITROGEN OXIDE (N2O4)
N2O4(L)	NITROGEN OXIDE (N2O4)
N2O5(G)	NITROGEN OXIDE (N2O5)
N3(G)	AZIDE (N3)
N4SI3(CR)	SILICON NITRIDE, ALPHA (SI3N4)
N5P3(CR)	PHOSPHORUS NITRIDE (P3N5)
O1(G)	OXYGEN (O)
O1+(G)	OXYGEN, ION (O+)
O1-(G)	OXYGEN, ION (O-)
O1PB1(CR)	LEAD OXIDE, RED (PBO)
O1PB1(CR)-B	LEAD OXIDE, YELLOW (PBO)
O1PB1(CR,L)	LEAD OXIDE (PBO)
O1PB1(G)	LEAD OXIDE (PBO)
O1PB1(L)	LEAD OXIDE (PBO)
O1P1(G)	PHOSPHORUS OXIDE (PO)
O1SI1(G)	SILICON OXIDE (SIO)
O1SR1(CR)	STRONTIUM OXIDE (SRO)
O1SR1(CR,L)	STRONTIUM OXIDE (SRO)
O1SR1(G)	STRONTIUM OXIDE (SRO)
O1SR1(L)	STRONTIUM OXIDE (SRO)
O1S1(G)	SULFUR OXIDE (SO)
O1S2(G)	SULFUR OXIDE (SSO)
O1TA1(G)	TANTALUM OXIDE (TAO)
O1TI1(CR)	TITANIUM OXIDE, ALPHA (TIO)
O1TI1(CR)-B	TITANIUM OXIDE, BETA (TIO)
O1TI1(CR,L)	TITANIUM OXIDE (TIO)
O1TI1(G)	TITANIUM OXIDE (TIO)
O1TI1(L)	TITANIUM OXIDE (TIO)
O1V1(CR)	VANADIUM OXIDE (VO)
O1V1(CR,L)	VANADIUM OXIDE (VO)
O1V1(G)	VANADIUM OXIDE (VO)
O1V1(L)	VANADIUM OXIDE (VO)
O1W1(G)	TUNGSTEN OXIDE (WO)
O1ZR1(G)	ZIRCONIUM OXIDE (ZRO)
O10P4(CR)	PHOSPHORUS OXIDE ((P2O5)2)
O10P4(G)	PHOSPHORUS OXIDE ((P2O5)2)
O12W4(G)	TUNGSTEN OXIDE ((WO3)4)
O2.72W1(CR)	TUNGSTEN OXIDE (WO2.72)
O2.90W1(CR)	TUNGSTEN OXIDE (WO2.90)
O2.96W1(CR)	TUNGSTEN OXIDE (WO2.96)
O2(REF)	OXYGEN (O2)
O2+(G)	OXYGEN, ION (O2+)
O2-(G)	OXYGEN, ION (O2-)
O2PB1(CR)	LEAD OXIDE (PBO2)
O2P1(G)	PHOSPHORUS OXIDE (PO2)

O2SI1(CR)	SILICON OXIDE, CRISTOBALITE, HIGH (SIO2)
O2SI1(CR)-B	SILICON OXIDE, CRISTOBALITE, LOW (SIO2)
O2SI1(CR)-C	SILICON OXIDE, QUARTZ (SIO2)
O2SI1(CR,L)	SILICON OXIDE (SIO2)
O2SI1(G)	SILICON OXIDE (SIO2)
O2SI1(L)	SILICON OXIDE (SIO2)
O2S1(G)	SULFUR DIOXIDE (SO2)
O2TA1(G)	TANTALUM OXIDE (TAO2)
O2TI1(CR)	TITANIUM OXIDE, ANATASE (TIO2)
O2TI1(CR)-B	TITANIUM OXIDE, RUTILE (TIO2)
O2TI1(CR,L)	TITANIUM OXIDE (TIO2)
O2TI1(G)	TITANIUM OXIDE (TIO2)
O2TI1(L)	TITANIUM OXIDE (TIO2)
O2V1(G)	VANADIUM OXIDE (VO2)
O2W1(CR)	TUNGSTEN OXIDE (WO2)
O2W1(G)	TUNGSTEN OXIDE (WO2)
O2ZR1(CR)	ZIRCONIUM OXIDE (ZRO2)
O2ZR1(CR,L)	ZIRCONIUM OXIDE (ZRO2)
O2ZR1(G)	ZIRCONIUM OXIDE (ZRO2)
O2ZR1(L)	ZIRCONIUM OXIDE (ZRO2)
O3(G)	OZONE (O3)
O3PB1SI1(CR)	LEAD SILICATE (PBSIO3)
O3S1(G)	SULFUR TRIOXIDE (SO3)
O3TI2(CR)	TITANIUM OXIDE (TI2O3)
O3TI2(CR,L)	TITANIUM OXIDE (TI2O3)
O3TI2(L)	TITANIUM OXIDE (TI2O3)
O3V2(CR)	VANADIUM OXIDE (V2O3)
O3V2(CR,L)	VANADIUM OXIDE (V2O3)
O3V2(L)	VANADIUM OXIDE (V2O3)
O3W1(CR)	TUNGSTEN OXIDE (WO3)
O3W1(CR,L)	TUNGSTEN OXIDE (WO3)
O3W1(G)	TUNGSTEN OXIDE (WO3)
O3W1(L)	TUNGSTEN OXIDE (WO3)
O4PB2SI1(CR)	LEAD SILICATE (PB2SIO4)
O4PB3(CR)	LEAD OXIDE (PB3O4)
O4SI1ZR1(CR)	ZIRCONIUM SILICATE (ZRSIO4)
O4S1ZN1(CR)	ZINC SULFATE (ZNSO4)
O4V2(CR)	VANADIUM OXIDE (V2O4)
O4V2(CR,L)	VANADIUM OXIDE (V2O4)
O4V2(L)	VANADIUM OXIDE (V2O4)
O5TA2(CR)	TANTALUM OXIDE (TA2O5)
O5TA2(CR,L)	TANTALUM OXIDE (TA2O5)
O5TA2(L)	TANTALUM OXIDE (TA2O5)
O5TI3(CR)	TITANIUM OXIDE, ALPHA (TI3O5)
O5TI3(CR)-B	TITANIUM OXIDE, BETA (TI3O5)
O5TI3(CR,L)	TITANIUM OXIDE (TI3O5)
O5TI3(L)	TITANIUM OXIDE (TI3O5)
O5V2(CR)	VANADIUM OXIDE (V2O5)
O5V2(CR,L)	VANADIUM OXIDE (V2O5)
O5V2(L)	VANADIUM OXIDE (V2O5)
O6P4(G)	PHOSPHORUS OXIDE ((P2O3)2)
O6W2(G)	TUNGSTEN OXIDE ((WO3)2)
O7TI4(CR)	TITANIUM OXIDE (TI4O7)
O7TI4(CR,L)	TITANIUM OXIDE (TI4O7)

O7TI4(L)	TITANIUM OXIDE (TI4O7)
O8W3(G)	TUNGSTEN OXIDE (W3O8)
O9W3(G)	TUNGSTEN OXIDE ((WO3)3)
PB1(CR)	LEAD (PB)
PB1(CR,L)	LEAD (PB)
PB1(G)	LEAD (PB)
PB1(L)	LEAD (PB)
PB1(REF)	LEAD (PB)
PB1+(G)	LEAD, ION (PB+)
PB1-(G)	LEAD, ION (PB-)
PB1S1(CR)	LEAD SULFIDE (PBS)
PB1S1(CR,L)	LEAD SULFIDE (PBS)
PB1S1(G)	LEAD SULFIDE (PBS)
PB1S1(L)	LEAD SULFIDE (PBS)
PB2(G)	LEAD (PB2)
P1(CR)	PHOSPHORUS, WHITE (P)
P1(CR)	PHOSPHORUS, RED, IV (P)
P1(CR)-B	PHOSPHORUS, RED, V (P)
P1(CR)-C	PHOSPHORUS, BLACK (P)
P1(CR,L)	PHOSPHORUS (P)
P1(G)	PHOSPHORUS (P)
P1(L)	PHOSPHORUS (P)
P1(REF)	PHOSPHORUS (P)
P1+(G)	PHOSPHORUS, ION (P+)
P1-(G)	PHOSPHORUS, ION (P-)
P1S1(G)	PHOSPHORUS SULFIDE (PS)
P2(G)	PHOSPHORUS (P2)
P4(G)	PHOSPHORUS (P4)
P4S3(CR)	PHOSPHORUS SULFIDE (P4S3)
P4S3(CR,L)	PHOSPHORUS SULFIDE (P4S3)
P4S3(G)	PHOSPHORUS SULFIDE (P4S3)
P4S3(L)	PHOSPHORUS SULFIDE (P4S3)
RB1(CR)	RUBIDIUM (RB)
RB1(CR,L)	RUBIDIUM (RB)
RB1(G)	RUBIDIUM (RB)
RB1(L)	RUBIDIUM (RB)
RB1(REF)	RUBIDIUM (RB)
RB1+(G)	RUBIDIUM, ION (RB+)
RB1-(G)	RUBIDIUM, ION (RB-)
RB2(G)	RUBIDIUM (RB2)
RN1(REF)	RADON (RN)
RN1+(G)	RADON, ION (RN+)
SI1(CR)	SILICON (SI)
1OO(CR,L)	SILICON (SI)
SI1(G)	SILICON (SI)
SI1(L)	SILICON (SI)
SI1(REF)	SILICON (SI)
SI1+(G)	SILICON, ION (SI+)
SI1-(G)	SILICON, ION (SI-)
SI2(G)	SILICON (SI2)
SI3(G)	SILICON (SI3)
SR1(CR)	STRONTIUM, ALPHA (SR)
SR1(CR)-B	STRONTIUM, BETA (SR)
SR1(CR,L)	STRONTIUM (SR)

SR1(G)	STRONTIUM (SR)
SR1(L)	STRONTIUM (SR)
SR1(REF)	STRONTIUM (SR)
SR1+(G)	STRONTIUM, ION (SR+)
S1(CR)	SULFUR, ORTHORHOMBIC (S)
S1(CR)-B	SULFUR, MONOCLINIC (S)
S1(CR,L)	SULFUR (S)
S1(G)	SULFUR (S)
S1(L)	SULFUR (S)
S1(REF)	SULFUR (S)
S1+(G)	SULFUR, ION (S+)
S1-(G)	SULFUR, ION (S-)
S1SI1(G)	SILICON SULFIDE (SIS)
S1SR1(CR)	STRONTIUM SULFIDE (SRS)
S1SR1(G)	STRONTIUM SULFIDE (SRS)
S2(G)	SULFUR (S2)
S2SI1(CR)	SILICON SULFIDE (SIS2)
S2SI1(CR,L)	SILICON SULFIDE (SIS2)
S2SI1(L)	SILICON SULFIDE (SIS2)
S3(G)	SULFUR (S3)
S4(G)	SULFUR (S4)
S5(G)	SULFUR (S5)
S6(G)	SULFUR (S6)
S7(G)	SULFUR (S7)
S8(G)	SULFUR (S8)
TA1(CR)	TANTALUM (TA)
TA1(CR,L)	TANTALUM (TA)
TA1(G)	TANTALUM (TA)
TA1(L)	TANTALUM (TA)
TA1(REF)	TANTALUM (TA)
TA1+(G)	TANTALUM, ION (TA+)
TA1-(G)	TANTALUM, ION (TA-)
TI1(CR)	TITANIUM, ALPHA (TI)
TI1(CR)-B	TITANIUM, BETA (TI)
TI1(CR,L)	TITANIUM (TI)
TI1(G)	TITANIUM (TI)
TI1(L)	TITANIUM (TI)
TI1(REF)	TITANIUM (TI)
TI1+(G)	TITANIUM, ION (TI+)
TI1-(G)	TITANIUM, ION (TI-)
V1(CR)	VANADIUM (V)
V1(CR,L)	VANADIUM (V)
V1(G)	VANADIUM (V)
V1(L)	VANADIUM (V)
V1(REF)	VANADIUM (V)
V1+(G)	VANADIUM, ION (V+)
V1-(G)	VANADIUM, ION (V-)
W1(CR)	TUNGSTEN (W)
W1(CR,L)	TUNGSTEN (W)
W1(G)	TUNGSTEN (W)
W1(L)	TUNGSTEN (W)
W1(REF)	TUNGSTEN (W)
W1+(G)	TUNGSTEN, ION (W+)
W1-(G)	TUNGSTEN, ION (W-)

```
XE1(REF)                      XENON (XE)
XE1+(G)                       XENON, ION (XE+)
ZN1(CR)                       ZINC (ZN)
ZN1(CR,L)                     ZINC (ZN)
ZN1(G)                        ZINC (ZN)
ZN1(L)                        ZINC (ZN)
ZN1(REF)                      ZINC (ZN)
ZN1+(G)                       ZINC, ION (ZN+)
ZN1-(G)                       ZINC, ION (ZN-)
ZR1(CR)                       ZIRCONIUM, ALPHA (ZR)
ZR1(CR)-B                     ZIRCONIUM, BETA (ZR)
ZR1(CR,L)                     ZIRCONIUM (ZR)
ZR1(G)                        ZIRCONIUM (ZR)
ZR1(L)                        ZIRCONIUM (ZR)
ZR1(REF)                      ZIRCONIUM (ZR)
ZR1+(G)                       ZIRCONIUM, ION (ZR+)
ZR1-(G)                       ZIRCONIUM, ION (ZR-)
```

APPENDIX D: THE JFIT PROGRAM

The JANAF tables (and hence the JANAF curvefit database) contain data for almost 1800 chemical species. Despite the broad scope of the tables, there are many circumstances in which a user will need to include one or more species in a SOLGASMIX data deck that are not available in the database. For this reason, the program JFIT was created. JFIT allows each user to keep his own auxilliary database of curvefits, which he can then reference any time from SOLGASMIX. The input data deck for JFIT is summarized below.

D.1: PUNCHING GUIDE FOR THE JFIT CURVEFITTING PROGRAM.

CARD	VARIABLE	DESCRIPTION
1.	NAME	Name of chemical species, up to 29 characters long. This name need not follow the Hill indexing conventions of the JANAF tables, and should not duplicate a species name already in the database.
	TITLE	A description of the species. Up to 50 characters long.

Note: Enclose both of the above character variables in single quotes. Separate them with a space or comma.

2.	HF	Heat of formation of species at 298 K. (KJ/MOLE).
3.	TEMP	Temperature (K)
	HH	$H(T)-H(298) = \int C_p dT$ The enthalpy change of heating the species from 298 K to TEMP. (KJ/MOLE)
	G	Gibbs free energy of at this temperature. (KJ/MOLE).

Note: $H(T)-H(298)$ and Gibbs free energy values must tabulated for at least 2 but not more than 75 different temperatures for each species. Each temperature corresponds to a separate card #3. In order to indicate the end of data for a given species, a negative temperature is entered. Up to 100 species can be contained in the user specified database (although more species could be added by making minor changes to the program). Note that the auxilliary database is replaced every time JFIT is run.

D.2: EXAMPLE DATA DECK FOR JFIT

The example data deck below contains thermochemical data for four species. The first two are imaginary species, with no heat of formation or Gibbs free energy at any temperature. These species are useful in rectifying certain error conditions (see Appendix A.3, and example #9 in Appendix B). The data for water allows one to run the second example in Appendix B.

```
'*(G)'      'UNOBTAINIUM'
0.00
298.15      0.0          0.00
2000.0      0.0          0.00
-100.0      0.0          0.00
'**(CR)'     'YOUCANTGETTIUM'
0.00
298.15   0.0          0.00
2000.0   0.0          0.00
-100.0   0.0          0.0
'WATER(L)'  'LIQUID WATER, UNDER 373.15 DEGREES'
-285.830
273.15            -1.884        -241.316
283.15            -1.130        -239.664
293.15            -0.376        -238.024
303.15            0.377         -236.392
313.15            1.130         -234.768
323.15            1.884         -233.158
333.15            2.638         -231.559
343.15            3.391         -229.965
353.15            4.146         -228.384
363.15            4.899         -226.810
373.15            5.653         -225.246
383.15            6.407         -223.689
-100.0            0.0            0.0
'H2O2(L)'    'HYDROGEN PEROXIDE, LIQUID'
-187.987
298.15   0.0       -120.563
300.0    0.163     -120.140
400.0    9.102     -98.009
431.0    11.874    -91.168
500.0    18.037    -75.902
600.0    26.967    -53.792
700.0    35.902    -31.635
800.0    44.832    -9.567
900.0    53.767    12.548
1000.0   62.697    34.663
1100.0   71.632    56.773
1200.0   80.562    78.888
1300.0   89.497    100.998
1400.0   98.432    123.113
1500.0   107.362   145.223
-100.0   0.        0.
```

APPENDIX E: SUBROUTINE JREAD

The JANAF curvefit database contains coefficients of fitted curves which accurately represent thermochemical data for nearly 1800 chemical species. For this reason, it was recognized that the usefulness of this database was not limited to SOLGASMIX applications, and that it would be appropriate to provide means for users to incorporate this data into their own applications programs.

Subroutine JREAD and the functions HFUN and GFUN provide the interface between FORTRAN programs and the database. JREAD must be called first: it reads the coefficients for ΔG and $H(T)-H(298)$ curvefits for any number of user specified species. JREAD also causes the coefficients and statistical data to be printed in a manner similar to that of SOLGASMIX (although no knowledge of SOLGASMIX is necessary to use this program).

After the call to JREAD, the functions HFUN and GFUN can be used to calculate the values of $H(T)-H(298)$ and ΔG, respectively for any of the previously specified species. The users guides below indicate the proper method of calling each of these subprograms. Appendix F contains a listing for the short application program JRACT, which uses JREAD, HFUN and GFUN to calculate values of ΔH_{rxn} and ΔG_{rxn} for any reaction.

The following syntax is used to call JREAD from a FORTRAN program:

```
    CALL JREAD(MS,MD,DLET,NAME,IFIL,GE,C,NOM,TOM,GTOM,
   *TMAX,HF,ERRMAX,ERMEAN,ERSTD,AMAXER,NPTS)
```

WHERE:

MS = The number of species for which thermochemical data is to be read from the database. (INTEGER)

MD = The dimension of the arrays defined below, exactly as defined in the calling program. This represents the maximum value which MS can take on, and as such must be greater than or equal to MS. (INTEGER)

DLET = A character variable representing the drive letter (A-E) which contains the curvefit data files and index files. This is only significant in the IBM PC version of JREAD, but must be specified for every operating system, as a dummy variable. (CHARACTER*1)

NAME = A character array with MD elements. This array contains the species names exactly as specified in the JANAF database Hill indexing notation, (or as specified by the user in his auxilliary auxilliary database- see Appendix D). Dimensioned as: CHARACTER*29 NAME(MD).

IFIL = The unit number for the file to which the coefficients and statistical data for the curvefits are to be written. Must be a valid FORTRAN unit number corresponding to a

file which has been opened in the calling
program (if IFIL = 6, most compilers
will write this data to the screen).

NOTE: JREAD reserves units 9,10, and 11. These units must
not be opened anywhere in an application from which
JREAD is called. IFIL cannot equal 9,10, or 11.

GE = An array of double precision curvefit coefficients
returned by JREAD for use with functions HFUN and
GFUN. Dimensioned as: REAL*8 GE(MD,2,8).

C = Another array of curvefit coefficients.
Dimensioned as: REAL*8 C(MD,6,3).

NOM = An integer array of MD elements. NOM(I) contains
the number of H(T)-H(298) curvefits for species
I. NOM has a maximum value of 3. Dimensioned as:
INTEGER NOM(MD).

TOM = A double precision array containing values for
the transition temperature from one H(T)-H(298)
curvefit to the next. Dimesioned as:
REAL*8 TOM(MD,3).

GTOM = A double precision array containing temperatures
of transition for those species with more than
one free energy curvefit. Dimesioned as:
REAL*8 GTOM(MD).

TMAX = An array containing values for the maximum temperature
for which the curvefits in the JANAF database are
valid. Dimensioned as REAL*8 TMAX(MD).

HF = An array returned by JREAD which contains the
heats of formation for each species. Values in
KJ/MOLE. Dimensioned as: REAL*8 HF(MD).

ERRMAX = An array containing the maximum errors on the
ΔG and H(T)-H(298) curvefits. ERRMAX values
are returned as percentages. For the I'th
species in the list, ERRMAX(I,1) is the maximum
percentage error on the Gibbs free energy curvefit,
while ERRMAX(I,2) is the maximum error on the
enthalpy curvefit. Dimensioned as REAL*8 ERRMAX(MD,2).

ERMEAN = An array containing values for the average percentage
error on the curvefits. See ERRMAX, above. Dimesioned
as: REAL*8 ERMEAN(MD,2).

ERSTD = An array containing the standard deviation of the
percentage error on the curvefits. REAL*8 ERSTD(MD,2).

AMAXER = An array containing values for the absolute value of

the maximum error on the thermochemical curvefits.
Both error terms are given in KJ/MOLE units.
Dimensioned as: REAL*8 AMAXER(MD,2).

NPTS = An integer array containing the number of data points
used to create the two curvefits. Again, the first
entry for each species corresponds to the Gibbs free
energy function, while the second represents the
enthalpy curvefit. INTEGER NPTS(MD,2).

E.1: FUNCTION HFUN

HFUN is a double precision FUNCTION subprogram which allows the calculation of values for H(T)-H(298); the integrated specific heat function: H(T) - H(298) (KJ/MOLE). JREAD must be called before HFUN. The calling syntax is:

```
HFUN(MD,C,TOM,NOM,T,I)
```

Where:

      I = The species number as defined in the calling arguments for JREAD. HFUN(MD,C,TOM,NOM,T,I) will correspond to H(T)-H(298) for the species who's chemical formula is NAME(I). (INTEGER).

      T = The temperature in Kelvin. (REAL*8).

And MD, C, TOM and NOM are as defined above for JREAD.

E.2: FUNCTION GFUN

GFUN is a double precision FUNCTION subprogram which allows the calculation of values for ΔG, the Gibbs free energy of formation of a species (KJ/MOLE). JREAD must be called before GFUN. The calling syntax is:

```
GFUN(MD,GE,GTOM,T,I)
```

Where:

      I = The species number as defined in the calling arguments for JREAD. (INTEGER).

      T = The temperature in Kelvin. (REAL*8).

And MD, GE, and GTOM are as defined above for JREAD.

APPENDIX F: THE JRACT PROGRAM

Included below is a listing and input example for the utility program
JRACT. This program was developed to demonstrate the use of subroutine
JREAD (see Appendix E) and the JANAF curvefit database for applications other
than SOLGASMIX. Some users will find it to be a useful program in its own right:
it calculates the free energy and enthalpy change for a chemical reaction
involving species from the JANAF curvefit database. Note that the program
below is set up to run on the PSU MVS system. Users will want to change the JCL
defining unit 11 to reflect their own userid and group number: Appendix H
contains a discussion of the correct form for the "SSS.GGGGGG.UUU" terms in
the listing below. JRACT is also available for the CMS and VAX/VMS operating
systems and the IBM PC. Appendix H is a discussion of the various systems for
which versions of the programs discussed in this work are available.

```
//MN2XXXXX JOB
// EXEC FVCG,LIB3='MEN.P66840.PNU.MODULES'
/*JOBPARM FULLSKIPS
//SYSIN DD *
        IMPLICIT REAL*8 (A-H,O-Z)
        CHARACTER*80 TITLE
        CHARACTER*29 NAME(50),NCHECK
        CHARACTER DLET
        DIMENSION NPTS(50,2),ERRMAX(50,2),ERMEAN(50,2),ERSTD(50,2),
       *AMAXER(50,2),HF(50),GTOM(50),TMAX(50),GE(50,2,8),NOM(50),
       *TOM(50,3),C(50,6,3),TEMP(50),XMOL(50)
C ***********************************************************
C    VARIABLES USED IN THIS PROGRAM:
C
C      NAME = AN ARRAY CONTAINING THE SPECIES NAMES.
C
C      NREAC = NUMBER OF REACTANTS.
C
C      NPROD = NUMBER OF PRODUCTS.
C
C      XMOL = AN ARRAY CONTAINING MOLAR AMOUNTS FOR EACH
C               SPECIES IN THE PROBLEM.
C
C      TEMP = AN ARRAY CONTAINING TEMPERATURE FOR EACH
C               SPECIES IN THE PROBLEM.
C
C       PHT = PRE HEAT- THE ENTHALPY CHANGE NECESSARY TO
C               HEAT THE REACTANTS TO THE REACTION TEMPERATURE.
C
C        HR = THE HEAT OF REACTION AT 298 K.
C
C      HEAT = TOTAL HEAT OF REACTION AT TEMPERATURE T.
C
C      HERR = ABSOLUTE MAXIMUM ERROR IN HEAT TERM.
C
C        GR = GIBBS FREE ENERGY CHANGE FOR THE REACTION.
C
C      GERR = ABSOLUTE MAXIMUM ERROR ON GR TERM.
```

```
      ELSE
          WRITE(IOUT,101) TITLE
      END IF
 100 FORMAT(T1,' ',A80//)
 101 FORMAT(T1,'1',A80//)
      WRITE(IOUT,300)
 300 FORMAT(' REACTANTS',T32,'MOLES',T44,'T (K)',T57,'H(T)-H(298)'
     *,T71,'DELTA G'/)
      DO 50 I=1,NREAC
      IF(TEMP(I).GT.298.2) THEN
         WRITE(IOUT,400) NAME(I),XMOL(I),TEMP(I),
     *HFUN(50,C,TOM,NOM,TEMP(I),I), GFUN(50,GE,GTOM,TEMP(I),I)
      ELSE
         WRITE(IOUT,400) NAME(I),XMOL(I),TEMP(I),
     *0.0D0,GFUN(50,GE,GTOM,TEMP(I),I)
      END IF
  50 CONTINUE
 400 FORMAT(' ',A29,T30,F7.3,T42,F7.2,T54,D12.5,T68,D12.5)
      WRITE(IOUT,500)
 500 FORMAT(//' PRODUCTS',T32,'MOLES',T44,'T (K)',T54,'H(T)-H(298)'
     *,T71,'DELTA G'/)
      DO 60 J=1,NPROD
         I=NREAC+J
         IF(TEMP(I).GT.298.2) THEN
         WRITE(IOUT,400) NAME(I),XMOL(I),TEMP(I),
     *HFUN(50,C,TOM,NOM,TEMP(I),I), GFUN(50,GE,GTOM,TEMP(I),I)
         ELSE
         WRITE(IOUT,400) NAME(I),XMOL(I),TEMP(I),
     *0.0D0,GFUN(50,GE,GTOM,TEMP(I),I)
         END IF
  60 CONTINUE
      WRITE(IOUT,600) HEAT,HERP
      WRITE(IOUT,700) GR,GERP
 600 FORMAT(//T10,' TOTAL HEAT OF REACTION  = ',D12.5,' KJ,  +/-  ',
     *F8.3,' %')
 700 FORMAT(/T10,' DELTA GIBBS FREE ENERGY = ',D12.5,' KJ,  +/-  ',
     *F8.3,' %')
      GOTO 70
  80 STOP
      END
//DATA.INPUT DD *
'EXAMPLE OF JRACT JOB. REACTION OF N2,H2 TO FORM NH3'
2,1
'N2(REF)'
'H2(REF)'
'H3N1(G)'
0.5    298.15
1.5    298.15
1.0    298.15
0.5    298.15
1.5    298.15
1.0    500.00
0.5    298.15
1.5    298.15
```

```
1.0    750.0
0.5    298.15
1.5    298.15
1.0   1000.00
//DATA.FT09F001 DD DSN=SSS.GGGGGG.UUU.JANAF.INX,
//     DISP=(OLD,KEEP),VOL=REF=SSS.GGGGGG.UUU.LIB,
//     DCB=(RECFM=FB,LRECL=88,BLKSIZE=19008)
//DATA.FT10F001 DD DSN=MEN.P66840.PNU.JANAF.DAT,
//     DISP=OLD,VOL=REF=MEN.P66840.PNU.LIB,
//     DCB=(RECFM=VBS,LRECL=68,BLKSIZE=19044)
//DATA.FT11F001 DD DSN=SSS.GGGGGG.UUU.AUX.DAT,
//     DISP=OLD,VOL=REF=SSS.GGGGGG.UUU.LIB,
//     DCB=(RECFM=VBS,LRECL=68,BLKSIZE=19044)
// EXEC PROMPTME
```

APPENDIX G: THE J-IND PROGRAM

Recent modifications to SOLGASMIX have greatly simplified the task of creating a data deck of parameters describing a specific chemical system. The use of the JANAF curvefit database allows one to utilize SOLGASMIX for a great many systems without ever having to look up thermochemical data for any chemical species. Unfortunately, the user is still faced with the task of entering the species names in correct Hill index notation, and correctly specifying the atomic composition of each species.

The utility program J-IND simplifies this somewhat tedious process by automatically creating the first portion of a SOLGASMIX data deck for any given problem. J-IND is available only on operating systems which support interactive processing, and prompts the user for all necessary input, using menus. The user is asked for a list of elements. The program then creates a list of species which contain those elements.

For use with SOLGASMIX, J-IND can be instructed to create a list of species which are composed <u>exclusively</u> of certain elements. This list can then be sorted by phase (which roughly groups the species in a manner compatible with the most common use of SOLGASMIX– gas phase first, then liquid species. followed by solid condensed phases). Finally, J-IND can be instructed to create a file with the species names specified in the correct format for entry into SOLGASMIX. This output file can then be edited to add the remaining control cards as specified in Appendix A.

This use of J-IND can significantly reduce the tedious work of manually poring over the index to the JANAF tables (as given in Appendix C), and has the added advantage that the user is unlikely to miss including a critical species in the data deck. Thus, the risk of overconstraining an equilibrium problem is considerably lessened (see the text for a discussion of this problem).

It should be noted that J-IND is useful in many situations beyond the creation of SOLGASMIX data decks. It is a general purpose indexing program for the JANAF tables, and allows the user to search the index automatically, extracting all species containing a given set of elements. In addition, the program allows one to sort a list of species by such factors as molecular weight, heat of formation, or composition.

APPENDIX H: OPERATING SYSTEM NOTES.

SOLGASMIX and its related utility programs are currently available for use on several computer systems. At Penn State, the program is available to users of the VM/CMS system on node PSUVM. In addition, the programs can be run in a non interactive mode using the MVS system, via any of the CMS nodes, RJE or INTERACT. A version of the program has been developed for the IBM personal computer (and compatibles). Finally, the mainframe SOLGASMIX program has been modified for use on DEC VAX/VMS minicomputers.

H.1: IBM VM/CMS OPERATING SYSTEM.

The version of SOLGASMIX running on CMS (20) supports all the interactive features recently added to the program. It is available at Penn State to all users who link to the minidisk containing the program and data files. The command to accomplish this is:

LAA PNU 101 RR (C

which creates a "C" minidisk for the user. Note that this disk must be attached as the C disk- users who routinely attach another minidisk as their C disk must first detach this disk to use SOLGASMIX. Note also that the above command gives read only privilege to a user. Those who wish to modify any of the programs on this disk must first copy them to a minidisk for which they have read-write access.

Because of space limitations, compiled versions of the various programs in the SOLGASMIX system have not been saved. The user must compile each program before he makes use of it. The proper format for the compile/link command is:

FVCL SOLG   (to create an executable SOLGASMIX module)
FVCL JFIT   (for JFIT: see Appendix D)
FVCL J-IND (for J-IND: see appendix G)
FVCL JRACT (for the JRACT example: see appendix F).

The user is advised to compile only those programs which he needs for a given session. The executable modules for these programs are quite large and can rapidly overwhelm all of one's available disk space.

When the SOLG, JFIT, or JRACT modules are executed, the user will be prompted for the file which contains the input data. The user must specify the complete file definition of the desired input file, including filename and filetype. The filemode usually need not be specified. The formats of these data files are described in Appendix A. Limited on line help is available by entering "HELP" instead of a filename. In addition, when running the SOLG or JFIT modules, the user can enter any valid FLIST (FileLIST) command at this prompt in order to view all available files. Each program also allows one to terminate program execution by entering "QUIT" instead of a filename. Of course, the above extensions imply that one cannot use "QUIT" "FLIST" or "HELP" as filenames for data decks to be used with any of these programs.

When using SOLG or JRACT, the user is asked to decide if he desires to see the program output on his screen or to have it written an output file. Entering "SCREEN" will cause all subsequent output to appear at the terminal. If this option is chosen, all output is spooled to the user's virtual reader as well as appearing on the screen. If SCREEN output is chosen when running JRACT, all of the curvefit coefficients and statistical data will be written to the file STAT LISTING E instead of appearing on the screen.

If it is desired to send output to a file (which preserves FORTRAN carriage controls) rather than viewing it at the terminal, the user should enter the filename of the desired output unit. Note that whenever any of these programs prompts for a desired output file name, only the filename should be entered. This file will be created with the file specification;

filename LISTING E.

The user is cautioned that these files all appear on his temporary minidisk and are erased every time he logs off.

One final feature of SOLGASMIX is that if the first letter of an output device name is given as a slash (/) character, the output will be split: the curvefit coefficients and statistical data will be sent to the file FT16F001 LISTING E, and the remainder of the data will be send to the screen (if "/SCREEN" is entered at the output device prompt) or to the desired file (if "/filename" is entered). This has the effect of reducing the amount of output which must be paged through at the terminal, or of cutting considerable amounts of output from the LISTING file. It is strongly recommended, however, that the user take time to examine the statistical data to determine all possible sources of inaccuracy in his SOLGASMIX analysis.

The formats of the various data files for use with the SOLG, JRACT or JFIT program modules is given elsewhere in this work. On CMS, the XEDIT editor is necessary to create these input files. Any files used for input to the various programs must have a fixed record format and 80 column logical record length. In almost all cases, these are the default settings for files created with XEDIT. If a file is inadvertently created with different parameters (which is occasionally the case for files which are transferred to CMS from another system), the XEDIT commands:

LRECL 80

and

RECFM F

will convert the file to the proper format.

Users wishing to use the JREAD, HFUN and GFUN subprograms in their own applications should transfer a copy of JRACT to their own minidisk and extract the necessary subroutines. Likewise, if it is desired to include activity coefficient information in a problem, the user will have to copy SOLGASMIX to his own disk and modify the FACTOR subprogram. One can also modify SUBROUTINE SPEQUA in order to perform additional calculations using the output from the program (SPEQUA is called after each equilibrium calculation).

The SOLGASMIX examples included in Appendix B are saved on the same minidisk as the program files, as EX01 DECK, EX02 DECK .... EX09 DECK. For some of these examples, it is necessary to first create an auxilliary (user specified) database of curve fits using the JFIT program (see Appendix D). The example given in Appendix D is saved as JFIT EXAMPLE on this same minidisk. Finally, the example of JRACT input given in Appendix F is saved as JRACT EXAMPLE. Running any or all of these examples is by far the best way to become familiar with the programs in the SOLGASMIX system.

H.2: IBM OS/VS2 (MVS) SYSTEM.

At Penn State, most batch processing is performed on the MVS system
(21). Batch jobs can be run on this system from either CMS, INTERACT or RJE.
Noninteractive versions of SOLGASMIX, JFIT, and JRACT are available. In order
to use any of the programs discussed below, it is first necessary to run a JFIT job,
which creates a customized version of the files JANAF.INX and AUX.DAT. A job
similar to the one below should be the first batch job run. This need only be done
once (although, of course, JFIT can be used many times to update the database
with other user defined species).

```
//MN2XXXXX JOB
// EXEC PGM=IEFBR14
//DELETE DD VOL=REF=SSS.GGGGGG.UUU.LIB,DISP=(OLD,DELETE),
// DSN=SSS.GGGGGG.UUU.JANAF.INX
//DELETE DD VOL=REF=SSS.GGGGGG.UUU.LIB,DISP=(OLD,DELETE),
// DSN=SSS.GGGGGG.UUU.AUX.DAT
// EXEC RUN,PROG=JFIT,LIB='MEN.P66840.PNU.MODULES'
/*JOBPARM FULLSKIPS
//DATA.FT11F001 DD DSN=MEN.P66840.PNU.MASTER.INX,
//    DISP=(OLD,KEEP),VOL=REF=MEN.P66840.PNU.LIB,
//    DCB=(RECFM=FB,LRECL=88,BLKSIZE=19008)
//DATA.FT12F001 DD DSN=SSS.GGGGGG.UUU.AUX.DAT,
//    DISP=(NEW,KEEP),VOL=REF=SSS.GGGGGG.UUU.LIB,
//    SPACE=(TRK,(5,5),RLSE),
//    DCB=(RECFM=VBS,LRECL=68,BLKSIZE=19044)
//DATA.FT13F001 DD DSN=SSS.GGGGGG.UUU.JANAF.INX,
//    DISP=(NEW,KEEP),VOL=REF=SSS.GGGGGG.UUU.LIB,
//    SPACE=(TRK,(5,5),RLSE),
//    DCB=(RECFM=FB,LRECL=88,BLKSIZE=19008)
//DATA.INPUT DD *
'*(G)'     'UNOBTAINIUM'
0.00
298.15      0.0          0.00
2000.0      0.0          0.00
-100.0      0.0          0.00
'**(CR)'    'YOUCANTGETTIUM'
0.00
298.15   0.0          0.00
2000.0   0.0          0.00
-100.0   0.0          0.0
'WATER(L)' 'LIQUID WATER, UNDER 373.15 DEGREES'
-285.830
273.15           -1.884          -241.316
283.15           -1.130          -239.664
293.15           -0.376          -238.024
303.15            0.377          -236.392
313.15            1.130          -234.768
323.15            1.884          -233.158
333.15            2.638          -231.559
343.15            3.391          -229.965
353.15            4.146          -228.384
```

```
363.15          4.899              -226.810
373.15          5.653              -225.246
383.15          6.407              -223.689
-100.0          0.0                 0.0
'H2O2(L)'   'HYDROGEN PEROXIDE, LIQUID'
-187.987
298.15   0.0      -120.563
300.0    0.163    -120.140
400.0    9.102    -98.009
431.0    11.874   -91.168
500.0    18.037   -75.902
600.0    26.967   -53.792
700.0    35.902   -31.635
800.0    44.832   -9.567
900.0    53.767   12.548
1000.0   62.697   34.663
1100.0   71.632   56.773
1200.0   80.562   78.888
1300.0   89.497   100.998
1400.0   98.432   123.113
1500.0   107.362  145.223
-100.0   0.       0.
// EXEC PROMPTME
```

An example of a SOLGASMIX job setup is shown below:

```
//MNWXXXXX JOB
// EXEC RUN,PROG=SOLG,LIB='MEN.P66840.PNU.MODULES'
/*JOBPARM FULLSKIPS
//DATA.FT09F001 DD DSN=SSS.GGGGGG.UUU.JANAF.INX,
//    DISP=(OLD,KEEP),VOL=REF=SSS.GGGGGG.UUU.LIB,
//    DCB=(RECFM=FB,LRECL=88,BLKSIZE=19008)
//DATA.FT10F001 DD DSN=MEN.P66840.PNU.JANAF.DAT,
//    DISP=OLD,VOL=REF=MEN.P66840.PNU.LIB,
//    DCB=(RECFM=VBS,LRECL=68,BLKSIZE=19044)
//DATA.FT11F001 DD DSN=SSS.GGGGGG.UUU.AUX.DAT,
//    DISP=OLD,VOL=REF=SSS.GGGGGG.UUU.LIB,
//    DCB=(RECFM=VBS,LRECL=68,BLKSIZE=19044)
//DATA.INPUT DD *
EX. 10: PU-C-O TEST RUN (SEE T.M. BESMANN ARTICLE).
 4 2 5 8 2
              'AR'        'PU'        'C'         'O'
'AR'          1.0         0.0         0.0         0.0
'CO'          0.0         0.0         1.0         1.0
'CO2'         0.0         0.0         1.0         2.0
'O2'          0.0         0.0         0.0         2.0
'PU'          0.0         1.0         0.0         0.0
'PUO'         0.0         1.0         0.0         1.0
'PUO2'        0.0         1.0         0.0         2.0
'PUC2'        0.0         1.0         2.0         0.0
'PUO'         0.0         1.0         0.0         1.0
'PUC'         0.0         1.0         1.0         0.0
```

```
'C'            0.0          0.0          1.0          0.0
'PU'           0.0          1.0          0.0          0.0
'PU2O3'        0.0          2.0          0.0          3.0
'PU2C3'        0.0          2.0          3.0          0.0
'PUC'          0.0          1.0          1.0          0.0
1 12 11 4
1
2 2 3
 0.0           0.0
-117290.      -84.39
-396220.      -0.13
0.0            0.0
 326800.      -88.83
-119000.      -41.0
-471100.       28.0
569000.      -210.0
-557330.       92.3
-32500.       -12.3
 0.0           0.0
 0.0           0.0
-1672000.     267.0
-164000.        7.84
-32500.       -12.3
 1900.
2
2
2 2 3 3
0.1
1.0
1.0         -0.1
0.1          0.05
12
// EXEC PROMPTME
```

Note that An example of a JRACT job is given in Appendix F.

Several changes may be necessary before these jobs will run correctly.
First, users of student (I) accounts must change the "MNW" in the first job card to
"STW" in order for the job category to be valid for their accounts. All
occurrences in JCL lines of the user specification "SSS.GGGGGG.UUU" must also
be changed. The "SSS" should either become "MEN" for non instructional
accounts, or "STU" for student accounts. "GGGGGG" should be changed to reflect
the correct group (account) number, and "UUU" should be changed to reflect the
proper userid. Finally, some jobs will not run correctly under category W. In this
case, users must change "MNW" to "MN1" or "STW" to "STI."

Two other short utility program were created for use on the batch
system. The JCL given below runs the program SUBSET, which allows one to copy
data pertaining to one or more species from the JANAF tape to an interact file.

```
//MN1XXXXX JOB
// EXEC PGM=IEFBR14
//DELETE DD VOL=REF=SSS.GGGGGG.UUU.LIB,DISP=(OLD,DELETE),
// DSN=SSS.GGGGGG.UUU.JANDAT
```

```
// EXEC RUN,PROG=SUBSET,LIB='MEN.P66840.PNU.MODULES'
/*JOBPARM FULLSKIPS
/*TAPE JANAFA,READ
//DATA.FT09F001 DD DSN=SSS.GGGGGG.UUU.JANAF.INX,
//    DISP=(OLD,KEEP),VOL=REF=SSS.GGGGGG.UUU.LIB,
//    DCB=(RECFM=FB,LRECL=88,BLKSIZE=19008)
//DATA.FT10F001 DD UNIT=TAPE,LABEL=(4,SL),DSN=THERMO,
//    VOL=SER=JANAFA,DISP=(OLD,KEEP),
//    DCB=(RECFM=FB,LRECL=85,BLKSIZE=31960)
//DATA.FT11F001 DD DSN=SSS.GGGGGG.UUU.JANDAT,
//    DISP=(NEW,KEEP),VOL=REF=SSS.GGGGGG.UUU.LIB,
//    SPACE=(TRK,(5,5),RLSE),
//    DCB=(RECFM=FB,LRECL=85,BLKSIZE=19040)
//DATA.INPUT DD *
AL1F6LI3(L)
K2O4S1(L)
ZR1+(G)
// EXEC PROMPTME
```

The second program, PRINTJAN, reads data from the JANDAT file (created by first running SUBSET), and prints it in a format similar to that of the bound version of the JANAF tables (using FORTRAN carriage controls).

```
//MN1XXXXX JOB
// EXEC RUN,PROG=PRINTJAN,LIB='MEN.P66840.PNU.MODULES'
/*JOBPARM FULLSKIPS
//DATA.FT11F001 DD DSN=SSS.GGGGGG.UUU.JANDAT,
//  DISP=(OLD,KEEP),VOL=REF=SSS.GGGGGG.UUU.LIB,
//  DCB=(RECFM=FB,LRECL=85,BLKSIZE=19040)
// EXEC PROMPTME
```

The examples given in this document are saved as members EX01, EX02 ... EX10, JFIT, JRACT, SUBSET, and PRINTJAN in the library:

$MEN.P66840.PNU.EXAMPLES.

INTERACT users can access these files by issuing commands of the form:

USE MEN.P66840.PNU.EXAMPLES(JFIT) ON VOL003

H.3: THE IBM PERSONAL COMPUTER.

A version of SOLGASMIX has been created which runs on the IBM Personal Computer (PC/XT/AT). This is a full implementation SOLGASMIX, with the exception that the maximum value NPKT can assume is 10. The program will operate on any PC which is compatible with the IBM PC, has 256 Kilobytes or more of RAM, and at least one disk drive. A hard disk drive is not necessary, but is strongly recommended, as it greatly reduces the time necessary to extract information from the curvefit database. An 8087 or 80287 math coprocessor chip is also highly recommended for large problems.

PC SOLGASMIX is well suited for use with problems that make a great deal of use of the interactive (menu driven) features. The author made use of the public domain library of assembly language routines created by Dudley Benton (22) in order to make the interactive features somewhat easier to use than in the VAX or CMS versions of SOLGASMIX.

Unfortunately, because of limitations inherent to the PC, very large systems can take a considerable amount of time to run. The equilibrium system containing C,H,O and N, given in the third example of Appendix B, is a case in point. This example was run on both a PC and AT, both with and without a numeric coprocessor. The run time (excluding disk access and I/O processes) for this problem are as follows:

    8 MHZ PC-AT with 80287 numeric coprocessor - 32.3 seconds
    STANDARD PC with 8087 numeric coprocessor - 50.8 seconds

    8 MHZ PC-AT w/o 80287 coprocessor - 239.0 seconds
    STANDARD PC w/o 8087 coprocessor - 773.0 seconds

The above values compare to a total execution time of 0.18 seconds for the CMS version of SOLGASMIX. Clearly, very large SOLGASMIX jobs should not be attempted on a PC without a numeric coprocessor. For smaller jobs, however, use of the personal computer is acceptable.

PC SOLGASMIX results are generally identical to those obtained with mainframe versions of the program. Some insignificant discrepancies between personal computer and mainframe/minicomputer versions, due to differences in double precision operations between MS FORTRAN (23) (as used on the PC), and IBM VS FORTRAN (24) or VAX FORTRAN (25). Note that since SOLGASMIX was linked with the MS FORTRAN "emulator" math package, the results of the program are just as accurate when run on personal computers without math coprocessors as when a machine containing an 8087 or 80287 is used.

The PC version of SOLGASMIX includes seven 5.25 inch diskettes. The contents of these diskettes are as follows:

    SOLGASMIX-PROGRAM: The executable module for SOLGASMIX
                          and the data file DRIVE.DAT.

       SOLG UTILITIES: Contains the PC version of the JFIT
                          program.

          EXAMPLES &   Includes the ten example data decks
          INSTRUCTIONS: discussed elsewhere in this work,

> as well as several additional examples.
> Also contains instructions for running
> the program.

J-IND: This disk contains the J-IND program and
data files.

JRACT/JREAD: Contains the JRACT program listing and
executable modules, and an object module
for subroutine JREAD, which can be linked
to other application programs.

DATA DISK 1/2: These two diskettes contain the JANAF
curvefit database and the auxilliary
(user specified) database created with
the JFIT program.

The file README.DOC, on the EXAMPLES diskette, contains information on
using SOLGASMIX from both diskette and hard disk based systems. In order to
obtain a hardcopy of these instructions, simply enter the command:

COPY README.DOC PRN

No previous experience with the IBM PC is required to use any of the programs
discussed above. However, most users will have a need to create data decks for
their own applications. For this reason, some familiarity with a word processor
or programming editor is required if one desires to use SOLGASMIX for problems
beyond those covered in the examples. The author uses KEDIT, which has the
advantage of emulating the CMS editor, making it easy to master for those
already familiar with XEDIT on IBM mainframes. The DOS line editor EDLIN can
also be used, as can more sophisticated wordprocessors which support a "non
document" or "DOS" mode for saving files.

H.4: THE VAX/VMS SYSTEM.

SOLGASMIX and its associated utility programs have been ported to a Digital Electronics VAX system. The VAX program operates in a manner similiar to the personal computer version. Note that the JANAF.DAT, AUX.DAT, and JANAF.INX files must be kept in the default directory along with the executable file SOLG.EXE. This requirement arises from the fact that the VMS operating system does not automatically search additional directories when a file is not found in the default (current) directory.

END

DATE

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